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	DESIGNATED/ELECTED OFFICE (DO/EO/US)										
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INT	TERNATIONAL APPLICATION NO.	PRIORITY DATE CLAIMED									
	PCT/GB00/03568 18 September 2000 17 September 1999										
TITLE OF INVENTION TARGET FOR ANTIVIRAL THERAPY											
APPLICANT(S) FOR DO/EO/US											
ANTSON, Alfred; MAITLAND, Norman Applicant herewith submits to the United States Designated/Elected Office (DO/EO/US) the following items and other information:											
	City and Cit										
l.		INT submission of items concerning a filing	under 35 U.S.C. 371.								
2.											
3.	This is an express request to begin national examination procedures (35 U.S.C. 371(f)). The submission must include items (5), (6), (9) and (21) indicated below.										
•		iration of 19 months from the priority date (Article 31).								
4. ~			· · · · · · · · · · · · · · · · · · ·								
5.		red only if not communicated by the Interna	tional Bureau).								
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		plication was filed in the United States Reco	eiving Office (RO/US).								
_		the International Application as filed (35 U									
6.	C	the international Application as free (55 C	3.3.1(0)(2)).								
	a. is attached hereto.	mitted under 35 U.S.C. 154(d)(4)									
_			19 (35 U.S.C. 371(c)(3))								
7.	7. Amendments to the claims of the International Application Under PCT Article 19 (35 U.S.C. 371(c)(3))										
	 a. are attached hereto (required only if not communicated by the International Bureau). b. have been communicated by the International Bureau. 										
		wever, the time limit for making such amen	dments has NOT expired.								
			unions has to respire								
	d. have not been made and		orticle 19 (35 U.S.C. 371(c)(3)).								
8.		the amendments to the claims under PCT A	THE 17 (33 C.S.C. 371(G)(3)).								
9.	An oath or declaration of the inven		v Evamination Report Under PCT								
10		the annexes of the International Preliminar	y Examination Report Shadi 1 0 2								
	Article 36 (35 U.S.C. 371(c)(5)).										
	Items 11 to 20 below concern docume										
1	. An Information Disclosure Statement under 37 CFR 1.97 and 1.98.										
١	2. An assignment document for recording. A separate cover sheet in compliance with 37 CFR 3.28 and 3.31 is included.										
	13. A FIRST preliminary amendment.										
Į	14. A SECOND or SUBSEQUENT preliminary amendment.										
1.5	15. A substitute specification.										
10	16. A change of power of attorney and/or address letter.										
	17. A computer-readable form of the sequence listing in accordance with PCT Rule 13ter.2 and 35 U.S.C. 1.821 - 1.825.										
	18. A second copy of the published international application under 35 U.S.C. 154(d)(4).										
11		guage translation of the international applica	tion under 35 U.S.C. 154(a)(4)								
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c. 🛚	The Commissioner is hereby authorized to charge any additional fees which may be required, or credit any overpayment to Deposit Account No. 50-0220. A duplicate copy of this sheet is enclosed.							
d. 🔲	Fees are to be charged to a credit card. WARNING: Information on this form may become public. Credit card information should not be included on this form. Provide credit card information and authorization on PTO-2038.							
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PATENT TRADEMARK OFFICE

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Date of Deposit: March 15, 2002
I hereby certify that this correspondence is being deposited with the United States Postal Service "Express Mail Post Office to Addressee" service under 37 CFR 1.10 on the date indicated above and is addressed to BOX PCT, Attn. DO/EO/US, Commissioner for Patents. Washington, DC 20231.

Susan E. Freedman

Attorney's Docket No. 9052-111

PATENT

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re:

Antson et al.

Examiner:

To be assigned

Serial No.:

PCT/GB00/03568

Group Art Unit:

To be assigned

Filed:

September 18, 2000

For:

Target for Antiviral Therapy

Date: March 15, 2002

Box PCT

U.S. Patent and Trademark Office

P.O. Box 2327

Arlington, VA 22202

Attn: DO/EO/US

PRELIMINARY AMENDMENT

Sir:

Prior to the examination of the above application, please amend the above referenced application as follows. Please enter the following amendments prior to the calculation of the filing fee. Pursuant to the rules for amendments under 37 C.F.R. §1.121, the claims have been amended herein using the rewritten claims format. The present amendment also includes a section entitled "VERSION WITH MARKINGS TO SHOW CHANGES MADE" attached hereto.

IN THE SPECIFICATION:

Please amend the specification as follows:

On page 1 after the title of the invention please add:

RELATED APPLICATIONS

This application claims priority under 35 U.S.C. § 371 from PCT/GB00/03568, (published under PCT Article 21(2) in English), filed on September 18, 2000, which claims priority to Great Britain Application Serial No. 9921938.8, filed on September 17, 1999, the disclosures of which are incorporated by reference herein in their entireties.

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IN THE CLAIMS:

Please enter the amended claims as follows:

- 2. (Amended) The E2NT dimer protein of Claim 1 wherein the residues lie on opposite sides of an N-terminal domain.
- 3. (Amended) The E2NT dimer protein of Claim 1, wherein the residues comprise a plurality of residue clusters associated with a structural role at an interface between N1 and N2 terminal domains of respective monomers within the dimer.
- 4. (Amended) The E2NT dimer protein of Claim 3 comprising three clusters.
- 5. (Amended) The E2NT dimer protein of Claim 3 wherein a first cluster of vital residues is associated with interactions between N1 and N2 domains and comprises any one or more of the following residues: Ile82, Glu90, Trp92, Lys112, Tyrl38, Val145.
- 6. (Amended) The E2NT dimer protein of Claim 3, wherein a second cluster of residues is associated with N1 interactions and comprises either or both of residues Trp33 and Leu94.
- 7. (Amended) The E2NT dimer protein of Claim 3, wherein a third cluster of residues is associated with N2 interactions and comprises any one or more of the following residues: Pro106, Lys111, Phel68, Trp134.
- 8. (Amended) The E2NT dimer protein of Claim 1, further comprising residues associated with transactivation and/or replication properties of E2.
- 9. (Amended) The E2NT dimer of Claim 8, wherein the residues comprise any one or more of the following residues: Glu20, Glu100, Asp122, Arg37, Glu39, Ile73, Gln12 and Ala69.

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10. (Amended) A method for determining the structure of a crystallised molecular

complex of an E2 N-terminal module (E2NT) dimer protein, wherein the E2NT dimer

protein and any of its mutations are mapped onto an E2 three-dimensional structure so

as to identify areas of amino acid conservation and the effect of mutations on folding

of the E2 protein.

11. (Amended) The method according to Claim 10 in rationalised antiviral drug

design.

12. (Amended) A method for identifying and/or selecting a candidate therapeutic

agent, the method comprising:

determining interaction of a E2 N-terminal module (E2NT) dimer in a sample

by contacting said sample with said candidate therapeutic agent and measuring DNA

loop formation in E2 in vitro.

13. (Amended) The method according to Claim 12 further comprising identifying

and/or selecting an antiviral candidate therapeutic agent.

14. (Amended) The method according to Claim 13, wherein the identifying and/or

selecting of the antiviral candidate therapeutic agent depends on its ability to interfere

with or block interactions of E2NT so as to interfere or block viral and/or cellular

transcription factors.

15. (Amended) A method of treating an HPV infection in a subject comprising:

introducing an E2NT dimerisation inhibitor in said subject.

16. (Amended) The method according to Claim 15 further comprising treating

warts, proliferative skin lesions and/or cervical cancer.

18. (Amended) Use of a dimerisation surface of an crystallised molecular complex

of an E2 N-terminal module (E2NT) dimer protein or homologue thereof according to

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Please cancel claim 33 without prejudice or disclaimer.

Please add the following new claims:

34. (New) A method for designing a potential antiviral compound for the prevention

or treatment of an HPV infection, comprising:

a) obtaining crystals of the E2NT dimer protein such that the three dimensional

structure of the crystallized E2NT dimer protein can be determined to a resolution of

about 1.9 Å or better,

b) evaluating the three dimensional structure of the crystallized E2NT dimer protein;

c) synthesizing the potential antiviral compound based on the three-dimensional

crystal structure of the crystallized E2NT dimer protein;

d) contacting an HPV virus with the potential antiviral compound; and

e) assaying the HPV virus for infectivity or monitoring the virus for activity, or both,

whereby a decrease in the infectivity of the virus or a change in the activity of the

virus indicates the compound may be used for the prevention or treatment of an HPV

infection.

35. (New) The method according to claim 34, wherein the antiviral compound is a

peptide or polypeptide.

36. (New) The method according to claim 34, wherein the E2 N-terminal module

dimer protein or homologue thereof comprises residues vital for transcriptional and

replication activities of said protein.

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37. (New) The method according to claim 36, wherein the residues comprise a plurality of residue clusters associated with a structural role at an interface between N1 and N2 terminal domains of respective monomers within the dimer.

38. (New) The method according to claim 37, wherein said E2NT dimer protein comprises three clusters.

39. (New) A method for designing a candidate compound for screening for binding to or inhibition of an HPV infection, comprising:

a) utilizing the three dimensional structure of a crystallized E2NT module dimer protein wherein the residues comprise a plurality of residue clusters associated with a structural role at an interface between N1 and N2 terminal domains of respective monomers within the dimer; and

b) designing a candidate binding compound based on the three-dimensional crystal structure of the crystallized E2NT dimer protein for binding to said dimer protein.

40. (New) The method of claim 39, wherein the candidate compound is a peptide or polypeptide.

41. (New) A method for determining the crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein, wherein the E2NT dimer protein and any of its mutations is mapped onto an E2 three-dimensional structure so as to identify areas of amino acid conservation and the effect of mutations on folding of the E2 protein.

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REMARKS

Please note that the claims pending at the time of this filing are the claims of the international application serial no. PCT/GB00/03568, *i.e.* claims 1-33. Claim 33 has been cancelled and claims 34-41 have been added. The pending claims have been amended above to better conform to United States practice. The marked-up version of the changes to the specification and claims are attached hereto in the "Version With Markings to Show Changes Made".

It is respectively submitted that this application is now in condition for substantive examination, which action is respectfully requested.

Respectfully submitted,

Jarett K. Abramson Attorney for Applicants Registration No. 47,376

Enc: Version With Markings to Show Changes Made

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Susan E. Freedman

Date of Signature: March 15, 2002

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VERSION WITH MARKINGS TO SHOW CHANGES MADE

IN THE CLAIMS:

The claims have been amended as follows:

- 2. (Amended) [An] <u>The E2NT dimer protein [according to] of Claim 1 wherein the residues lie on opposite sides of an N-terminal domain.</u>
- 3. (Amended) [An] <u>The E2NT dimer protein [according to either preceding claim] of Claim 1</u>, wherein the residues comprise a plurality of residue clusters associated with a structural role at an interface between N1 and N2 terminal domains of respective monomers within the dimer.
- 4. (Amended) [An] <u>The E2NT dimer protein [according to] of Claim 3 comprising three clusters.</u>
- 5. (Amended) [An] <u>The E2NT dimer protein [according to either of Claims] of Claim</u> 3 [or 4] wherein a first cluster of vital residues is associated with interactions between N1 and N2 domains and comprises any one or more of the following residues: Ile82, Glu90, Trp92, Lys112, Tyrl38, Val145.
- 6. (Amended) [An] <u>The E2NT dimer protein [according to any one of Claims 3-5] of Claim 3</u>, wherein a second cluster of residues is associated with N1 interactions and comprises either or both of residues Trp33 and Leu94.
- 7. (Amended) [An] <u>The E2NT dimer protein [according to any one of Claims 3-6] of Claim 3,</u> wherein a third cluster of residues is associated with N2 interactions and comprises any one or more of the following residues: Pro106, Lys111, Phel68, Trp134.
- 8. (Amended) [An] <u>The E2NT dimer protein [according to any preceding claim]</u> of <u>Claim 1</u>, further comprising residues associated with transactivation and/or replication properties of E2.

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9. (Amended) [An] <u>The E2NT dimer [according to] of Claim 8</u>, wherein the residues comprise any one or more of the following residues: Glu20, Glu100, Asp122, Arg37, Glu39, Ile73, Gln12 and Ala69.

- 10. (Amended) [Use of a] A method for determining the structure of a crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein, [according to any preceding claim or homologue thereof in mapping mutations] wherein the E2NT dimer protein and any of its mutations are mapped onto an E2 three-dimensional structure so as to identify areas of amino acid conservation and the effect of mutations on folding of the E2 protein.
- 11. (Amended) [Use] <u>The method</u> according to Claim 10 in rationalised antiviral drug design.
- 12. (Amended) [An *in vitro*] <u>A</u> method for identifying and/or selecting a candidate therapeutic agent, the method comprising:

determining interaction of a E2 N-terminal module (E2NT) dimer in a sample by contacting said sample with said candidate therapeutic agent and measuring DNA loop formation in E2 *in vitro*.

- 13. (Amended) [Use of the] <u>The</u> method according to Claim 12 [in] <u>further</u> <u>comprising</u> identifying and/or selecting an antiviral candidate therapeutic agent.
- 14. (Amended) [Use according to] The method according to Claim 13, wherein [identification/selection] the identifying and/or selecting of the antiviral candidate therapeutic agent depends on its ability to interfere with or block interactions of E2NT so as to interfere or block viral and/or cellular transcription factors.
- 15. (Amended) [Use of an E2NT dimerisation inhibitor for the preparation of a medicament for treatment of conditions that arise as a result of] A method of treating an HPV infection in a subject comprising:

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introducing an E2NT dimerisation inhibitor in said subject.

16. (Amended) [Use] <u>The method</u> according to Claim 15 [for the treatment of] <u>further comprising treating</u> warts, proliferative skin lesions and/or cervical cancer.

18. (Amended) Use of a dimerisation surface of an crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein or homologue thereof according to [any one of Claims 1-9] <u>Claim 1</u> as a target site for interaction with putative antiviral agents and/or for measuring efficacy of said agents.

- 20. (Amended) [A] <u>The</u> method of claim 19, wherein the method by which the E2NT crystal structure is obtainable comprises crystallisation using hanging-drop vapour diffusion.
- 21. (Amended) [A] The method of claim 19, [or claim 20] wherein the method by which E2NT crystal structure is obtainable comprises X-ray diffraction using uranium acetate and gold cyanide E2NT derivatives and refining with data extending to 1.9 Å spacing.
- 22. (Amended) [A] <u>The</u> method of [any of claims] <u>Claim</u> 19 [to 21], wherein the crystal structure comprises the portions of amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94.
- 23. (Amended) [A] <u>The</u> method of [any of claims] <u>Claim</u> 19 [to 22], wherein the rationalised drug design comprises designing drugs which interact with the dimerisation surface of E2NT.
- 32. (Amended) A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex [according to claim 27 or claim 28] comprising a dimerisation surface defined by structure coordinates of E2NT amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94 according to Table 3 or a homologue of said molecule or

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molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å, comprising the steps of:

- a. employing computational means to perform a fitting operation between the chemical entity and a dimerisation surface of the molecule or molecular complex; and
- b. analysing the results of said fitting operation to quantify the association between the chemical entity and the dimerisation surface.

Claim 33 has been canceled without prejudice or disclaimer.

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Target for Antiviral Therapy

The present invention provides a crystallised module of a nuclear phosphoprotein and an assay and method for determining interactions with human papillomavirus E2 for use in drug design, for use particularly but not exclusively in designing antiviral algents with potential use in treating warts, proliferative skin lesions and carcinoma of the cervix.

Background to the Invention

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Human papillomaviruses (HPVs) cause warts and proliferative lesions in skin and other epithelia. In a minority of HPV types ("high risk", which include HPVs 16, 18, 31, 33, 45 and 56), further transformation of the wart lesions can produce tumours, most notably carcinoma of the cervix. HPVs have evolved a sophisticated system of control, mediated by protein:DNA and protein:protein interactions, that involves both cellular and viral proteins. The 45 kDalton nuclear phosphoprotein, E2, has two central roles in this control. It acts as the principal virally encoded transcription factor and, in association with the viral E1 protein, it creates the molecular complex at the origin of the viral DNA replication².

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E2 has three distinct modules. The N-terminal module (E2NT) of about 200 amino acids is responsible for interactions with viral and host cell transcription factors. It is followed by a flexible, proline-rich, linker module and a C-terminal module (E2CT), each of about 100 amino acids ³ (Fig. 1a). The E2CT binds as a homodimer to DNA sites with a consensus sequence of ACCGN₄CGGT ⁴. In most HPVs a long upstream regulatory region (URR) precedes the viral genes and contains four spatially conserved E2 binding sites: three sites proximal to the transcription start site (p97 in HPV16) and one approximately 500bp upstream.

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The dimer of E2CT serves to anchor E2 protein to its recognition sites on the DNA, the function of the E2NT is to bind and localise at least three cellular transcription

factors, Sp1, TFIIB and AMF-1, to the transcription initiation complex. In addition, E2 interacts with another viral protein, E1, which has ATPase and helicase activities. E1 itself binds to the viral origin of replication which consists of about 100 bp and is surrounded by the three E2-binding sites, proximal to the transcription start. The E2:E1 interaction greatly increases the rate of HPV genome replication^{2,5,6}, Fig. 1a. An intact E2 is essential for the normal productive (wart) life cycle of HPV, however during malignant progression HPV DNA is integrated into the host cell genome, which usually results in disruption of the E2/E1 ORFs and loss of E2 protein, in turn leading to dysregulated expression of the viral oncogenes E6 and E7⁷.

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Consistent with its role as a transcription regulator, E2 has been shown to direct the formation of loops in DNA containing E2 binding sites⁸. The loops were only formed with intact E2, and not with the E2CT alone. The E2 binding sites did not function independently and their co-operative effect was mediated by full length E2, leading the authors to suggest that there were specific interactions mediated by E2 that bridged across the set of DNA binding sites through its N-terminal. A similar DNA loop structure could also be achieved with Sp1, a cellular transcription factor, which forms a complex with distally bound E2 ⁹; Sp1/E2 interactions are critical for transcription activation in BPV¹⁰.

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Eighty six known E2 proteins from different species and different human subtypes¹¹ are highly conserved, with sequence identities typically of 35% in the N and C-terminal modules (Fig. 1b). The crystal structure of the E2CT has been determined both alone and in complex with cognate DNA¹²⁻¹⁴. The module is a dimer with a barrel fold, and induces substantial bending (42-44°) of the DNA from its B-form double helix¹⁴.

The structure of the proteolytic fragment of HPV18 E2NT, missing 65 N-terminal residues, was recently reported at 2.1 Å spacing¹⁵. This allowed some analysis of mutational effects on function, although the missing 65 amino acids contain residues which are essential for the transcriptional and replication activities of the protein.

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We report herein the structure of the complete E2NT determined by X-ray analysis at 1.9 Å. We have found that it is an L-shaped molecule with the residues vital for transcriptional and replication activities of the protein lying on opposite sides of the N-terminal domain. Surprisingly, our results show that the surface, vital for transcription activation, is in fact involved in association of two E2NT's into a dimer. We suggest that dimerisation of E2NT plays an important and key role in induction of DNA loop formation, the mechanism by which distally bound transcription factors would be brought close to the site of transcription initiation. More importantly, our results raise the possibility that dimer formation serves as a molecular switch between early gene expression and viral genome replication during HPV infection.

The process of rationalised drug design requires no explanation or teaching for the skilled person but a brief description is given here of computational design for the lay reader: various computational analyses are necessary to determine whether a molecule is sufficiently similar to the target moiety or structure. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., Waltham, Mass.) version 3.3, and as described in the accompanying User's Guide, Volume 3 pages. 134-135.

The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses a least squares fitting algorithm that computes the optimum translation and

rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

One skilled in the art may use one of several methods to screen chemical entities or fragments for their ability to associate with a target. Again, these methods require no elucidation for the skilled person but are described here for the benefit of the unskilled reader. The screening process may begin by visual inspection of the target on the computer screen, generated from a machine-readable storage medium.

Selected fragments or chemical entities may then be positioned in a variety of orientations, or docked, within that binding pocket as defined supra. Docking may be accomplished using software such as Quanta and Sybyl, followed by energy minimization and molecular dynamics with standard molecular mechanics force fields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical entities. These include:

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- GRID (P. J. Goodford, "A Computational Procedure for Determining Energetically
 Favorable Binding Sites on Biologically Important Macromolecules", J. Med. Chem.,
 pp. 849-857 (1985)). GRID is available from Oxford University, Oxford, UK.
 - 2. MCSS (A. Miranker et al., "Functionality Maps of Binding Sites: A Multiple Copy Simultaneous Search Method." Proteins: Structure, Function and Genetics, 11, pp. 29-34 (1991)). MCSS is available from Molecular Simulations, Burlington, Mass.
 - 3. AUTODOCK (D. S. Goodsell et al., "Automated Docking of Substrates to Proteins by Simulated Annealing", Proteins: Structure, Function, and Genetics, 8, pp. 195-202 (1990)). AUTODOCK is available from Scripps Research Institute, La Jolla, Calif.

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4. DOCK (I. D. Kuntz et al., "A Geometric Approach to Macromolecule-Ligand Interactions", J. Mol. Biol., 161, pp. 269-288 (1982)). DOCK is available from University of California, San Francisco, Calif.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or complex. Assembly may be preceded by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of calcineurin. This would be followed by manual model building using software such as Quanta or Sybyl.

Useful programs to aid one of skill in the art in connecting the individual chemical entities or fragments include:

- CAVEAT (P. A. Bartlett et al, "CAVEAT: A Program to Facilitate the Structure Derived Design of Biologically Active Molecules". In Molecular Recognition in Chemical and Biological Problems", Special Pub., Royal Chem. Soc., 78, pp. 182-196 (1989)). CAVEAT is available from the University of California, Berkeley, Calif.
- 2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif). This area is reviewed in Y. C. Martin, "3D Database Searching in Drug Design", J. Med. Chem., 35, pp. 2145-2154 (1992).
 - 3. HOOK (available from Molecular Simulations, Burlington, Mass.).

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As the skilled reader will already know, instead of proceeding to build ligand for the target in a step-wise fashion, one fragment or chemical entity at a time as described above, inhibitory or other target-binding compounds may be designed as a whole or *de novo*. These methods include:

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1. LUDI (H.-J. Bohm, "The Computer Program LUDI: A New Method for the De Novo Design of Enzyme Inhibitors", J. Comp. Aid. Molec. Design, 6, pp. 61-78 (1992)). LUDI is available from Biosym Technologies, San Diego, Calif.

- 5 2. LEGEND (Y. Nishibata et al., Tetrahedron, 47, p. 8985 (1991)). LEGEND is available from Molecular Simulations, Burlington, Mass.
 - 3. LeapFrog (available from Tripos Associates, St. Louis, Mo.).
- Other molecular modelling techniques may also be employed. See, e.g., N. C. Cohen et al., "Molecular Modeling Software and Methods for Medicinal Chemistry, J. Med. Chem., 33, pp. 883-894 (1990). See also, M. A. Navia et al., "The Use of Structural Information in Drug Design", Current Opinions in Structural Biology, 2, pp. 202-210 (1992).

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Once a compound has been designed or selected by the above methods, the efficiency with which that entity may bind to a target may be tested and optimized by computational evaluation. For example, an effective ligand will preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient ligands should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, preferably, not greater than 7 kcal/mole. Ligands may interact with the target in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free entity and the average energy of the conformations observed when the inhibitor binds to the protein.

An entity designed or selected as binding to a target may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target enzyme. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole

interactions. Specifically, the sum of all electrostatic interactions between the inhibitor or other ligand and the target, when the inhibitor is bound to the target, preferably make a neutral or favourable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C [M. J. Frisch, Gaussian, Inc., Pittsburgh, Pa. .COPYRGT.1992]; AMBER, version 4.0 [P. A. Kollman, University of California at San Francisco, .COPYRGT.1994]; QUANTA/CHARMM [Molecular Simulations, Inc., Burlington, Mass. .COPYRGT.1994]; and Insight II/Discover (Biosysm Technologies Inc., San Diego, Calif. .COPYRGT.1994). These programs may be implemented, for instance, using a Silicon Graphics workstation, IRIS 4D/35 or IBM RISC/6000 workstation model 550. Other hardware systems and software packages will be known to those skilled in the art.

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Once the ligand has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components known in the art to alter conformation should be avoided. Such substituted chemical compounds may then be analyzed for efficiency of fit to a calcineurin-like binding pocket by the same computer methods described in detail, above. Again, all these facts are familiar to the skilled person.

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Another approach is the computational screening of small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to a target. In this screening, the quality of fit of such entities to the binding site may be judged either by shape complementarity or by estimated interaction energy. E. C. Meng et al., J. Comp. Chem., 13, pp. 505-524 (1992).

The computational analysis and design of molecules, as well as software and computer systems therefor are described in US Patent No 5,978,740 which is included herein by reference, including specifically but not by way of limitation the computer system diagram described with reference to and illustrated in Fig 3 thereof as well as the data storage media diagram described with reference to and illustrated in Fig 4s and 5 thereof.

Statement of the Invention

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According to a first aspect of the invention there is provided a crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein or homologue thereof, for use in rationalised drug design. We have found that the dimer comprises residues vital for transcriptional and replicational activities of said protein lying on opposite sides of an N-terminal domain, for use in rationalised drug design.

Preferably the E2NT dimer protein is substantially as depicted in any of Figures 2c and/or 3a-d.

According to a second aspect of the invention there is provided an *in vitro* method for identifying and/or selecting a candidate therapeutic agent, the method comprising determining interaction of a E2 N-terminal module (E2NT) dimer in a sample by contacting said sample with said candidate therapeutic agent and measuring DNA loop formation.

25 Preferably, the method is for use in identifying and/or selecting an antiviral candidate therapeutic agent.

Preferably, the candidate therapeutic agent interferes or blocks interactions of E2NT so as to interfere or block viral and/or cellular transcription factors.

According to a third aspect of the invention there is provided use of an E2NT dimerisation inhibitor in the preparation of a medicament for use in treating warts, proliferative skin lesions and/or cervical cancer.

According to a fourth aspect of the invention there is provided a method of monitoring the efficacy of an antiviral therapy in a patient receiving a medicament for the treatment of warts, proliferative skin lesions and/or cervical cancer comprising taking a sample from said patient and measuring E2NT interactions and/or DNA loop formation.

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Thus it will be appreciated that a patient can be monitored at the start of therapy to test its effectiveness. Alternatively, a patient can be monitored once a therapy has been established so as to monitor its efficacy with a view to altering a therapy if found to be unsatisfactory.

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The human papillomavirus E2 protein controls the primary transcription and replication of the viral genome. Both activities are governed by a ~200 amino acid N-terminal module (E2NT) which is connected to a DNA binding C-terminal module by a flexible linker. The crystal structure of the E2NT module from high-risk type 16 human papillomavirus reveals an L-shaped molecule with two closely packed domains, each with a novel fold. It forms a dimer in the crystal and in solution. The dimer structure is important in the interactions of E2NT with viral and cellular transcription factors and is the key to induction of DNA loops by E2. These loops may serve to target distal DNA-binding transcription factors to the region proximal to the start of transcription. The structure has implications for antiviral drug design and cervical cancer therapy.

The invention includes method for identifying and/or selecting a candidate therapeutic agent, comprising applying rationalised drug design to a crystal structure obtainable by crystallising E2NT, cryogenically freezing the crystals and generating the crystal structure using X-ray diffraction. The method by which the E2NT crystal

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structure is obtainable may comprise crystallisation using hanging-drop vapour diffusion. The method by which E2NT crystal structure is obtainable may comprise X-ray diffraction using uranium acetate and gold cyanide E2NT derivatives and refining with data extending to 1.9 Å spacing. The crystal structure may comprise the portions of amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94. The rationalised drug design may comprise designing drugs which interact with the dimerisation surface of E2NT.

Further provided is a computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises or a three-dimensional representation of a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, wherein said computer comprises:

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(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of E2NT amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94 according to Table 3;

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(b) a working memory for storing instructions for processing said machine-readable data;

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- (c) a central-processing unit coupled to said working memory and to said machinereadable data storage medium for processing said machine readable data into said three-dimensional representation; and
- (d) a display coupled to said central-processing unit for displaying said threedimensional representation.

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In class of embodiments, the three-dimensional representation is of a molecule or molecular complex is defined by the set of structure coordinates according to Table 3, or wherein said three-dimensional representation is of a homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5 Å.

An additional aspect of the invention resides in a computer for determining at least a portion of the structure coordinates corresponding to an X-ray diffraction pattern of a molecule or molecular complex, wherein said computer comprises:

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- (a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates according to Table 3;
- 15 (b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises an X-ray diffraction pattern of said molecule or molecular complex;
- (c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);
 - (d) a central-processing unit coupled to said working memory and to said machinereadable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and
 - (e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.
- 30 A yet further aspect of the invention relates to a crystallised molecule or molecular complex comprising a dimerisation surface defined by structure coordinates of E2NT

amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94 according to Table 3or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å. The molecule or molecular complex may be defined by the set of structure coordinates according to Table 3, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

27. A machine-readable data storage medium (e.g. a magnetic or optical storage medium, for example a hard disc, a floppy disc or a CD-ROM), comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising a dimerisation surface defined by structure coordinates of E2NT amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94 according to Table 3, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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In the machine-readable data storage medium the molecule or molecular complex may be defined by the set of structure coordinates according to Table 3, or a homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than

25 1.5Å.

The invention further provides a machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second

set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates according to Table 3; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex.

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In another aspect, the invention resides in a method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex according to the invention, comprising the steps of:

- 10 a. employing computational means to perform a fitting operation between the chemical entity and a dimerisation surface of the molecule or molecular complex; and
 - b. analysing the results of said fitting operation to quantify the association between the chemical entity and the dimerisation surface.

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Detailed Description of the Invention

The invention will now be described by way of example only with reference to the following Figures and Tables wherein:

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Table 1 illustrates X-ray data and phasing statistics;

Table 2 illustrates refinement and model correlation;

10 Table 3 shows the structure coordinates of the E2NT module;

Figure 1a represents functional assignments of HPV 16 E2 protein;

Figure 1b illustrates sequence alignment of E2NT modules from a subset of HPV types;

Figure 2a illustrates a stereo view of electron density with a final model at the dimer interface of the E2NT module, viewed down the crystallographic two-fold axis;

20 Figure 2b represents a stereo ribbon diagram of the E2NT module;

Figure 2c represents the E2NT dimer;

Figure 3a illustrates a schematic view of URR;

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Figure 3b illustrates a schematic view of loop formation induced by binding of E2 proteins to two cognate sites;

Figure 3c illustrates a model of E2 dimer formation;

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Figure 3d illustrates loops within URR as shown in Figure 3b;

Figure 4a illustrates the distribution of conserved residues on the E2NT monomer;

Figure 4b illustrates a first cluster of conserved residues on the E2NT monomer;

Figure 4c illustrates a second cluster of conserved residues on the E2NT monomer; and

Figure 4d illustrates conserved residues Gln12 and Glu39.

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Those of skill in the art understand that a set of structure coordinates for an enzyme or an enzyme-complex or a portion thereof, is a relative set of points that define a shape in three dimensions. Thus, it is possible that an entirely different set of coordinates could define a similar or identical shape. Moreover, slight variations caused by acceptable errors in the individual coordinates will have little, if any effect on overall shape. In terms of binding pockets, these acceptable variations would not be expected to alter the nature of ligands that could associate with those pockets.

The term "associating with" refers to a condition of proximity between a chemical entity or compound, or portions thereof, and a calcineurin molecule or portions thereof. The association may be non-covalent--wherein the juxtaposition is energetically favored by hydrogen bonding or van der Waals or electrostatic interactions--or it may be covalent.

The invention is also described with reference to US Patent No 5,978,740 which is included herein by reference, including specifically but not by way of limitation the computer system diagram described with reference to and illustrated in Fig 3 thereof as well as the data storage media diagram described with reference to and illustrated in Fig s 4 and 5 thereof.

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With reference to Figure 1a and functional assignments of E2. There is shown in a schematic view of NT, linker and CT modules of E2 indicating known functions of each module. Amino acid numbers which delimit the modules correspond to E2 from HPV16. In Figure 1b, there is shown the sequence alignment of the E2NT modules from a subset of HPV types (HPV16, HPV18, HPV11 and HPV2a) and one BPV type. Shaded blocks above the alignment indicate the experimentally determined secondary structure. Shaded blocks below the sequences indicate the minimal peptide sequences involved in protein:protein interactions, suggested by mutation studies. Residues with more than 90% identity among 86 PV types are coloured: red for internal structural residues, green for residues within the fulcrum region, blue for surface residues.

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With reference to the structural features of E2, in Figure 2a there is shown a stereo view of the electron density with the final model, at the dimer interface of the E2NT module, viewed down the crystallographic two-fold axis. The likelihood weighted map is contoured at the 1.5 σ level. Ribbons of two independent monomers are coloured blue and yellow. Side chains of ARG37 and Ile73 which are known to be critical for transactivation ^{4,31}, are shown in dark green; side chain of other residues at the dimer interface are shown in light green. Oxygen atoms are in red, nitrogen in blue, water molecules are shown as orange spheres and hydrogen bonds as dashed sticks. In Figure 2b, there is shown a stereo ribbon diagram of the E2NT module. The N1 domain is shown in aquamarine and the N2 domain in pink, with the fulcrum in green. In Figure 2c, there is shown the dimer of E2NT, showing the extent of the interface between the two subunits. The view is as in Figure 2a but rotated clockwise by 90°. Side chains of Gln12 and Glu39 which are critical for interactions with E1 ^{31-33,37} are shown in magenta. Side chains of residues at the dimer interface are coloured as per Figure 2a.

With reference to Figures 3a-d there is shown loop formation in the URR of HPV16. In Figure 3a, there is shown a schematic view of the URR. The four E2-binding sites are represented by boxes. Numbers in italics indicate distances between individual

sites upstream of the p97 promoter. Two possible E2 configurations, with separate or dimeric E2NT modules are shown. In Figure 3b, there is shown a schematic view of loop formation induced by binding of E2 proteins to two cognate sites, based on the experiments reported by Knight *et al*⁸. In Figure 3d, there is shown the possible DNA loops within the URR as depicted in Figure 3b. In Figure 3c, there is shown a model of the formation of E2 dimers, showing interactions between both the C-terminal and E2NT modules. The C-terminal dimer, with its bound DNA, is based on the crystal structure of this module¹². The E2NT dimer is proposed from the present work. The relative orientation and position of the E2NT and C-terminal modules is purely schematic.

With reference to Figures 4a-d there are shown functionally important residues. In Figure 4a, there is shown the distribution of conserved residues on the E2NT monomer. In Figures 4b and 4c there is shown the two clusters of conserved residues in the fulcrum of E2NT. In Figure 4d, there are shown conserved residues Gln12 and Glu39. Bonds in ball-and stick models are coloured aquamarine (N1 domain), pink (N2 domain) and green (fulcrum). Hydrogen bonds are shown as dashed lines, water molecules as orange spheres, oxygen atoms are in red, nitrogen atoms in blue and sulphur atoms in yellow.

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There is convincing evidence that the E2 protein has an extended structure, is flexible and that its functions depend on this property. This is probably the reason why the intact protein has not yet been crystallised in spite of intensive efforts. A major problem is the extended flexible linker module, with around 100 residues. E2NT proved difficult to crystallise, and a number of different constructs were made and overexpressed before crystallisation with residues 1 to 201 was achieved, but even this construct possessed limited stability. The protein had to be crystallised within 2-3 days of purification; crystals grew within about 48 hours but only retained useful diffraction quality for a further 2-3 days. This necessitated that crystals be rapidly vitrified in cryoprotectant buffer and stored for use as soon as detector time became available ¹⁶.

Crystals of E2NT belong to the space group P3₁21 with unit-cell dimensions a=b=54.3 Å, c=155.5 Å. The structure was determined using two heavy atom derivatives and refined with data extending to 1.9 Å spacing (Fig. 2a). The main chain is well defined throughout with the exception of residues 125 and 126 which are in an exposed loop and are mobile. There was density for the last residue of the His-tag at the N-terminus, but none for the remainder of this entity. All amino acids lie in the allowed regions of the Ramachandran (ϕ, ψ) plot¹⁷ with 92.4% in most favoured regions¹⁸.

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The transactivation module is composed of two domains, N1 and N2, arranged so as to give it an overall L-shaped appearance. Analysis of the PDB¹⁹using DALI²⁰shows that both have unique organisation of their secondary structures. Domain N1, which forms the N-terminus of the intact E2, is composed of residues 1 to 92, which fold into three long α -helices, Figure 2 (b,c). There is a tight loop between $\alpha 1$ and $\alpha 2$ and a more extended one between $\alpha 2$ and $\alpha 3$. The three helices pack antiparallel to one another in the form of a twisted plane, with angles of about 20° and 25° between the pairs of consecutive helices. DALI indicated a maximum Z-score of 5.7, that could suggest a significant correlation, for colicin la, a membrane protein which contains three 80 Å long α -helices arranged more or less coplanar²¹. This is the only other known protein that contains a true domain made up of such a packing of three helices. In addition there were 42 other structures which gave Z-scores above 4.0, most of which were four helix bundles, such as bacterioferritin²². However, in these only two of the three N1 helices superimposed simultaneously on two, not always adjacent, bundle helices as a result of a more planar arrangement of helices within N1. The indications are that the similarities observed reflect the optimum stacking angle of antiparallel helices against one another rather than suggesting a common ancestor for the evolution of these molecules.

Domain N2 is made up of residues 110 to 201 and is composed almost entirely of antiparallel β structure, with only one short helical segment from residues 171 to 178,

Figure 2 (b,c). The secondary structure has two short three and four stranded antiparallel β pleated sheets interconnected by two stranded β ribbons. For this domain DALI failed to identify any significant homologies to known structures, with a highest Z-score of only 2.1. From the analysis of Harris and Botchan¹⁵ and the present study, the N2 fold appears to be novel.

The structure between the N1 and N2 domains (residues 93 to 109) contains two consecutive single turns of helical structure, resulting in a compact and tight turn. It packs closely against elements of both domains and is not a truly independent structural domain. Rather it forms a fulcrum in the L-shape formed by N1 and N2 where it could act as a hinge, allowing the two domains to change their relative conformation in a specific way. Several of the interactions between adjacent regions of chain in the fulcrum are mediated indirectly through H-bonds involving water molecules, suggesting the possibility of flexibility.

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One of the most striking features of the crystal structure is the association of two E2NT monomers into a tight dimer. The two E2NT monomers pack around the crystallographic 2-fold axis, as shown in Figure 2a. The dimer interface is formed mostly by amino acids from helices $\alpha 2$ and $\alpha 3$ of the N1 domain and by residues 142-144 from the N2 domain. The total buried surface area between the two E2NT is 2026 A° , comparable to the 2444 A° buried between the two E2CT¹², which are known to form a tight dimer with a K_d of 3-6 x 10⁻⁸ M ^{23,24}.

In the E2NT dimer interface, each subunit contributes a cluster of seven equivalent residues, invariant or conserved in the 86 known sequences of E2¹¹, with many direct and water-mediated hydrogen bonds and rather few non-polar contacts, Fig. 2. Analysis of the dimer forming surfaces shows that all the direct hydrogen bonds between monomers are made through these seven amino acids. For the invariant Arg37, all possible side-chain hydrogen bonds are madé and all are well defined, Figure 2. Three of them are across the dimer interface. One hydrogen bond is critical, from NH2 to the main chain carbonyl oxygen of Leu77. A second hydrogen bond from NH2 is to OG1 of Thr81; in five out of 86 sequences this residue is

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glutamine, and modelling shows a hydrogen bond is possible to the NE of Arg37. The NH1 of Arg71 H-bonds to the OE1 of residue 80, which is Glu or Gln in all but six variants. At the NE of Arg37 there is an ideal H-bond to water that itself makes another strong H-bond across the dimer interface to the main-chain carbonyl oxygen of residue 142. The role of the invariant Ile73 is the filling of the intersubunit nonpolar volume made up of the aliphatic parts of Arg37, Gln76 and of Leu77 - in this case from both monomers. The Leu77 is in a few sequences substituted by valine or isoleucine and in 9 out of 86 known sequences by methionine. Inspection of the structure shows that Leu77 is partially exposed to the solvent and therefore different hydrophobic side chains could be easily accommodated at this site. important non-polar side chain is Ala69. Its side chain methyl packs into the surface of the other monomer at van de Waals distance from the main chain of residue 142. The only observed mutation of Ala69 is to Gly, and is easily accommodated. Gln76 is conserved or has homologous substitutions in about 2/3 of E2 sequences; in about 1/4 of the sequences there is methionine or valine at this position¹¹. Although hydrophobic substitutions of Gln76 would disrupt the hydrogen bonding to Glu80 across the dimer interface, and to Arg37 from the same subunit, the hydrophobic side chain at residue 76 could instead make a compensating hydrophobic interaction with the adjacent intersubunit hydrophobic pocket formed by Ile73 and Leu77.

Modelling of the amino acid variations in the 86 known papillomavirus E2 proteins into the other contacts at the dimer interface shows that they generally can be accommodated (data not shown). The consistency of the hydrogen bonds and van de Waals contacts at the monomer-monomer interface in the various sequences suggests therefore that the E2NT dimer interactions are potentially present in all papillomaviruses.

The first experimental evidence for the E2NT dimerisation in the presence of DNA with multiple E2-binding sites was provided by Knight et al in 1991⁸. Their studies showed that intact E2 led to the formation of DNA loops on templates with widely separated E2 binding sites, while a truncated E2, containing the DNA-binding E2CT but missing the N-terminal 161 residues, did not. Such dimerisation is further

supported by the observed synergistic transcription activation by a complex of two DNA-bound E2 dimers²⁵.

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To analyse the functional behaviour of the E2NT dimers further, we measured the analytical sedimentation equilibrium using by dissociation constant ultracentrifugation of recombinant E2NT protein containing the 201 N-terminal amino acids. A value of $K_d = 8.1 \pm 4 \times 10^{-6}$ M was obtained, indicating mediumstrength association. The micromolar range of the E2NT dimer K_d is certainly physiologically significant, and compares well with values for other transcription factors which have relatively low dissociation constants, often with the K_d values between 1 µM and 20 µM ^{26,27}. In vivo, the interaction could be enhanced when the two E2NT modules are placed in close proximity. Indeed, E2CT forms dimers which bind to the multiple DNA-binding sites located within the URR of viral DNA with K_d of protein: DNA interactions usually in the nanomolar range²⁸. Consequently, the local concentration of E2NT, bound to the E2CT via the non-conserved, flexible ~80 amino-acid linker, is effectively increased.

E2NT dimer interactions, as seen in the crystal structure, could form either between modules which are already part of a single E2 dimer, formed as a result of E2CT dimerisation interactions and bound to a single E2 binding site on the DNA (Fig. 3a), or between two preformed E2 dimers located on different E2 binding sites (Fig. 3b). The results of the electron microscopy suggest that the latter dimerisation does occur⁸. Although no direct experimental evidence exists for the former dimerisation, it does also seem possible due to the flexibility of the linker connecting the two modules. We propose that E2 molecules may initially keep their N-terminal modules within their internal dimers, but swap N-terminal modules and cross link to E2 molecules bound to distant DNA binding sites to form active loop structures during transcriptional activation and / or HPV DNA replication (Figure 3d). As discussed below, the effects of mutations on transcriptional transactivation can be explained in terms of the dimer being an essential element in this process.

E2 is a regulator of both transcription and viral DNA replication and thus interacts with other viral and host macromolecules in the infected cell. Indication of the possible importance of individual residues in the function comes firstly from the structure, secondly from the extensive set of sequences of the papillomaviral E2's and thirdly from mutagenesis studies on the individual proteins. In the following we make a primary attempt to map the molecule's function onto its structure.

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The pattern of amino acid conservation for the 86 available papilloma sequences¹¹ has been analysed using the GCG program suite²⁹. The sequences exhibit striking variation, characteristic of some virus families. However, 33 of the total 201 residues in the E2NT construct were totally or highly conserved. Fig. 4a illustrates the distribution of these 33 residues in the dimer. These were categorised into two sets: those with an essentially structural role and those exposed on the surface with a potential for intermolecular interactions. Thirteen residues (Fig. 1b) are buried or play a purely structural role within the monomer, they are not expected to be of functional importance and will not be discussed here.

A further 12 of these 33 residues stand out as having a structural role in the interface of the N1 and N2 domains. They form three clusters, the first making direct interactions between the two domains (Ile82, Glu90, Trp92, Lys112, Tyr138, Val145) and two separate sets of interactions, one from N2 (Pro106, Lys111, Phe168, Trp134) and the other from N1 (Trp33, Leu94) to the structure connecting them, referred to here as a fulcrum. The first two clusters are shown in Figure 4 b, c and it can be seen that Lys111 and Lys112 play key roles. Their side chains point in opposite directions to one another and their terminal amino groups are involved in near ideal patterns of hydrogen bonds. The flat surfaces of their extended side chains stack against Trp134 and Trp92, respectively. This clustering of invariant residues at the interface indicates a functional importance for the relative orientation of N1 and N2. The fulcrum could indeed provide a flexible pivot between the two domains, but there is no direct evidence for this as yet. Finally, while the side chain of Glu90 is held tightly in place by two H-bonds and could have a structural role, its OE2 atom is

exposed on the surface and is surrounded by near invariant side-chains, which may thus play a part in interactions with other molecules.

Of the remaining eight conserved residues, mutational substitutions of Glu20, Glu100 and Asp122 ³⁰⁻³³ had moderate effects on the transactivation and replication properties of E2, which depended on a particular viral strain. Glu20 lies on the top surface of N1. Asp122 lies far away on the distal surface of N2. Glu100 is completely exposed and points into the solvent at the junction of the L between the N1 and N2 domains. The functional role of these amino acids has yet to be clarified.

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Three conserved amino acids (Arg37, Glu39 and Ile73) have been subjected to point mutation and the effects on the two principal functions of E2, i.e. transactivation and HPV DNA replication have been assessed (reviewed in⁴,also ^{31,34,35}). Together with the remaining two conserved amino acids, Gln12 and Ala69, these residues form two functionally important surfaces (see below).

Finally, a number of the mutational results (reviewed in ⁴, also ^{31,34,35}) correspond to residues that can be assigned to structural roles. Substitution of these residues will lead to substantial conformational changes and a probable inability to fold correctly. This is particularly true for some of the deletion mutants involving the core of the molecule. Knowledge of the structure will allow a more rational choice and design of mutants in the future.

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The induction of DNA loops by E2NT dimerisation could be important for the construction of the active transcription bubble by targeting DNA-binding transcription factors, bound at distal sites, to the region proximal to the start of transcription (reviewed in ³⁶). In support of this, residues Arg37, Ile73 and Gln76 map onto the surface of E2NT involved in dimer formation, and mutations result in considerable disruption of transactivation, while having little effect on replication, ^{4,15,31}. The structure also shows that Ala69 which points its side chain methyl across the dimer interface, is also critical for transactivation. Mutational substitutions to

amino acids with longer side chains should have a knock out effect on E2NT dimer formation and consequently on transactivation.

The sites of association with cellular transcription factors AMF-1 (residues 74-134) and TFIIB (134-216) were previously mapped onto the E2NT module (Figure 1) using a series of deletion mutants as well as point mutations^{34,35}. These sites were mutually exclusive. In the structure, residues 74-134 include the fulcrum, while residues 134-216 correspond to domain N2. Further biochemical and structural studies can now be planned to characterise these interactions in more detail.

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Replication of the viral genome is initiated by binding of another viral protein, E1, to the origin of DNA replication⁴ which is itself flanked by two E2 binding sites, Fig. 3a. While the function of E2CT dimers is to bind specifically to the DNA sites, E2NT interaction with E1 enhances the binding of E1 to this region. Mutational substitutions of Glu39 generally retained transcriptional activation while DNA replication was substantially reduced^{31-33,37}. In the structure, the conserved Glu39 makes every possible hydrogen bond by its side chain carboxyl oxygens, Fig. 4d. One hydrogen bond is to NE2 of Gln12, which is absolutely conserved in all known sequences of E2. The other three hydrogen bonds are to the water molecules which are part of an intimate net of well-defined water molecules surrounding Glu39 and mediating its interactions with adjacent residues. Interestingly, a number of these protein interactions with water molecules are conserved as they are made to the protein backbone, including carbonyl oxygens of Gln12, Met36 and Lys68. While mutation of Gln12 in BPV1 only slightly affected both transactivation and replication, it substantially reduced cooperative origin binding^{30,32}. positioning of Gln12 and Glu39 in the three-dimensional structure further enhances the notion that these two resides are involved in interactions with E1. The conserved set of interactions at Gln12/Glu39 suggests that the main chain carbonyl oxygens of Gln12 and Met36 and the conserved water molecules could be also involved in these interactions. Gln12/Glu39 are surrounded by Leu8, Ile15, Met36, Tyr43, Gln57 and

Lys68, which are unlikely to contribute into E2/E1 interactions, as these residues are not well conserved in E2 sequences from different papillomaviruses.

The Gln12/Glu39 cluster lies on a side of the N1 domain which is opposite to the side involved in transactivation (and dimerisation), Figure 2c. Notably, the spatial separation of the two functionally important surfaces suggests that E2NT module could be able to interact with E1 at the same time as it interacts through the dimerisation interface with another E2NT module.

The structure reported here for the entire E2 transactivation module, has several implications for understanding of E2 function. It is now possible to map known mutations onto the E2 three-dimensional structure, and to use the knowledge of amino acid conservation and the effects of mutations to assign roles in folding, structure and function to residues. To this end, our results indicate that molecular surfaces involved in transactivation and E1-binding are located at opposite sides of the N1 domain of E2NT, suggesting that both surfaces could be accessed simultaneously by other protein factors. In line with these observations, E1 has been shown to modulate transactivation by directly interacting with E2, leading to repression of transactivation in the presence of excess E1³⁸. It is not inconceivable that the docking of E2NT dimer with E1 is sufficient to block further association with other target proteins.

The structure shows that the transactivation surface is involved in the formation of the E2NT dimer, which could cross-link E2 molecules bound by their E2CT modules to well-separated DNA sites. Inevitably, such dimerisation would cause DNA to form a loop structure, targeting distally bound transcription factors to regions close to the promoter. While this process has been suggested to be essential for transactivation³⁶, the definition of interacting surfaces between E2 and other cellular transcription factors requires a great deal of further study.

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Our results suggest that the process of DNA loop formation could involve swapping of E2NT modules across E2 dimers bound at separated DNA sites (Fig. 3a-d). The polar components of the monomer-monomer interactions may favour such exchange. Domain swapping is a well-recognised phenomenon that occurs relatively frequently between two individual monomers containing domains connected by a flexible linker ^{39,40}. E2 is to our knowledge the first example where the swapping event is predicted to occur between dimers.

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The dimerisation surface of E2 represents a good target for designing anti-viral drugs, since it is essential for viral transcription, there is no homologous human protein and the residues forming the interface are highly conserved among different viral strains. Dynamic interactions between transcription factors play a central role in the regulation of transcription and replication. Dimerisation, heterodimerisation and the monomer-to-dimer transition may play important roles during the control of the papillomavirus life cycle. These processes themselves can be regulated through phosphorylation, proteolysis, interaction with small ligands or changes in their intracellular concentration. It has been suggested that E2 can regulate the switch between early gene expression and viral genome replication during HPV infection⁴¹. It is possible that dimerisation of E2NT modules plays an essential role during this process. One scenario would be to activate transcription via induction of DNA loop formation at early stages of the viral life cycle. At later stages, when the concentration of expressed E2 proteins within the cell becomes high and comparable with the K_d for E2 dimer formation, free E2NT modules could compete for dimerisation with those involved in DNA loop formation and titrate them away, switching off transcription and stimulating replication. It is also possible that other protein factors could be involved in this process, including, for example, E1.

The invention therefore includes the use of E2NT crystal structure in the design of anti-viral drugs, since it is essential for viral transcription. In the rationalised computational design of drugs using the crystal structure, computational analyses are therefore necessary to determine whether a molecule or the E2NT-binding portion

thereof is sufficiently similar to the E2NT structure. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., Waltham, Mass.) version 3.3, and as described in the accompanying User's Guide, Volume 3 pages. 134-135.

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The Molecular Similarity application permits comparisons between different structures, different conformations of the same structure, and different parts of the same structure. The procedure used in Molecular Similarity to compare structures is divided into four steps: 1) load the structures to be compared; 2) define the atom equivalences in these structures; 3) perform a fitting operation; and 4) analyze the results.

Each structure is identified by a name. One structure is identified as the target (i.e., the fixed structure); all remaining structures are working structures (i.e., moving structures). Atom equivalency within QUANTA is defined by user input and, for the purpose of this invention equivalent atoms may be defined as protein backbone atoms (N, C.alpha., C and O) for all conserved residues between the two structures being compared. We will also consider only rigid fitting operations.

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When a rigid fitting method is used, the working structure is translated and rotated to obtain an optimum fit with the target structure. The fitting operation uses a least squares fitting algorithm that computes the optimum translation and rotation to be applied to the moving structure, such that the root mean square difference of the fit over the specified pairs of equivalent atom is an absolute minimum. This number, given in angstroms, is reported by QUANTA.

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For the purpose of one class of embodiments this invention, any set of structure coordinates of a molecule or molecular complex that has a root mean square deviation of conserved residue backbone atoms (N, C.alpha., C, O) of less than 1.5 .ANG. when superimposed—using backbone atoms—on the relevant structure coordinates of E2NT are considered identical. More preferably, the root mean square

deviation is less than 1.0 .ANG.. Most preferably, the root mean square deviation is less than 0.5 .ANG..

The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein from the backbone of E2NT a dimerising portion thereof, for example as defined by the structure coordinates of E2NT described herein.

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The term "least squares" refers to a method based on the principle that the best estimate of a value is that in which the sum of the squares of the deviations of observed values is a minimum.

15 Materials and Methods

Purification and crystallisation.

Details of the purification and crystallisation of E2NT have been described previously¹⁶. Briefly, the ORF encoding the N-terminal 201 residues of HPV-16 E2 was cloned into the prokaryotic expression plasmid pET15b downstream of the 20-residue His-tag leader sequence; protein was expressed in *E. coli*BL21(DE3)pLysS and purified using nickel affinity and anion exchange chromatography. Crystals were obtained by hanging drop vapour diffusion with 0.8-1.2M ammonium sulphate, 0.1M triethanolamine pH 8.0-8.3 and 3-5% 2-methyl-2,4-pentanediol. Crystals grew only with very fresh protein preparations and deteriorated in terms of diffraction quality in less than a week. This necessitated freezing and storage of crystals in liquid nitrogen immediately after growth, as discussed above.

Structure determination.

All data were recorded on cryogenically frozen crystals. A native crystal was frozen for which initial data were recorded to 3.4 Å¹⁶. For the screening of derivatives,

crystal stability was even more limiting. Nine crystals were soaked in various heavy atom reagents immediately after growth. The crystals were screened in-house using a MAR research imaging plate on a Rigaku RU200 rotating anode source, by recording 3° of data for each and analysing the fractional isomorphous difference from the native. Three derivatives showed promising differences from the native, in the range of 15-20% after scaling using SCALEPACK⁴² and were stored in liquid nitrogen. The native crystal was transported to EMBL Hamburg where 1.9 Å data were measured using synchrotron radiation from beam line X11, Table 1. In addition data were recorded at EMBL for the three promising derivatives to about 2.7 Å. Two of these derivatives proved useful in phase determination and the structure was solved by multiple isomorphous replacement with anomalous scattering (MIRAS) at 2.7 Å. The two derivatives were solved independently using the CCP4 suite 43 from the difference Patterson synthesis and by direct methods as implemented in SHELX44. Both contained a single heavy atom site. Phases, calculated using MLPHARE, were enhanced by solvent flattening45 using a solvent content of 50 %. The resulting high quality density map was easily interpretable and the initial model was built using QUANTA (Molecular Simulations) for all but four residues of the construct, ignoring the His-tag. The model was completed with REFMAC (resolution 20-1.9 Å) using a bulk solvent correction, to an R-factor of 23.3 % (R_{Free} 29.7 % - for 5 % of the data). There are 221 residues in the recombinant protein: the first twenty comprise the His-Tag. The final model contains all but two of the 201 residues of the real protein: residues 125-126 are disordered and lie in a flexible surface loop. Only one residue, His0, of the His-tag has clear density and an ordered conformation. In addition there are 187 water molecules, which were selected using ARP46during the course of refinement. The main statistics of the refined model are shown in Table 2.

Analytical ultracentrifugation.

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Experiments were carried out in an Optima XL-A ultracentrifuge (Beckman-Coultier, 30 CA, USA) using scanning UV optics. During the experiments, the recombinant E2NT was in 10mM TrisHCl pH 8.0, 5mM DTT, 0.2 mM EDTA, 300 mM NaCl.

Data were obtained at rotor speeds of 12,000 and 16,000 rpm, and the time to equilibrium was 10-12 hours. All runs were carried out at 293K, and all radial scans were at a wavelength of 280 nm. Dissociation constants were obtained by nonlinear regression using the Beckman ultracentrifuge software.

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Table 1
X-ray data and phasing statistics

•						
Data set	Native	UAc	AuCN			
Space Group	P3 ₁ 21	P3 ₁ 21	P3121			
a ,b (Å)	54.68	54.49	54.58			
c (Å)	155.73	155.66	156.50			
Resolution (Å)	30-1.9	20-2.7	20 - 2.7			
Temperature, K	120	120	120			
Wavelength (Å)	0.86	0.86	0.86			
Unique reflections	21751	7873	7937			
Completeness (%)	98.8 (89.3)	99.8 (96.1)	99.7 (93.8)			
(outer shell)						
R-merge (outer shell)	0.058 (0.339)	0.073 (0.271)	0.061 (0.268)			
Phasing Power: (centric	/ acentric)	1.55 / 2.07	0.95 / 1.40			
FOM: MIRAS		0.59				
FOM: DM 20-2.7 Å (2.	.7 - 1.9 Å)	0.88 (0.61)				
DM: Mean phase chang	ge (20-2.7 Å)	32 °				
R-factor (FreeR)	0.223 (0.295)					

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Table 2
Refinement and model correlation

	Resolution		1.9 – 10.0 Å
	Number of protein atoms		1622
5	Number of solvent sites		211
	Number of reflections used in refinement		20637
	Number of reflections used for Rfree calculation	1111	
	R-factor ‡		0.232
	Rfree ‡		0.305
10	Average atomic B-factor*, Å ²	protein atoms	38.0
		water molecules	48.5
	R.m.s. deviations from ideal geometry (Å). Targets	in parentheses	
		bond distance	0.013 (0.020)
	•	angle distance	0.026 (0.040)
15		chiral volume	0.142 (0.200)

 $[\]label{eq:crystallographic R-factor} \begin{tabular}{l} \updownarrow Crystallographic R-factor, $R_{(free)} = $\sum ||F_o| - |F_c|| / \sum |F_o| \ . \end{tabular}$

20 Table 3

	CRYST	. .	680	54.6	80 155.	730 90.00 90.00	120.00 P3121
	SCALE1	54.		1829	0.01056	0.00000	0.00000
25	SCALE1			0000	0.02112	0.00000	0.00000
2,5	SCALE3			0000	0.00000	0.00642	0.00000
	ATOM	1	N.O	HIS A		5.469 -26.512	52.262 1.00 61.92
	ATOM	2	CA	HIS A	-	6.434 -25.669	51.568 1.00 61.84
	ATOM	3	C	HIS A		6.263 -25.743	50.051 1.00 53.91
30	ATOM	4	ŏ	HIS A		6.089 -24.713	49.607 1.00 69.59
	ATOM	5	СВ	HIS A			51.965 1.00 54.18
	ATOM	6	CG	HIS A		7.848 -26.468	53.431 0.00 99.00
	ATOM	7	ND1	HIS A	. 0	7.914 -25.533	54.412 0.00 99.00
	MOTA	8	CD2	HIS A	0	7.732 -27.728	54.027 0.00 99.00
35	ATOM	9	CE1	HIS A	. 0	7.828 -26.215	55.570 0.00 99.00
	ATOM	10	NE2	HIS A	0	7.723 -27.531	55.370 0.00 99.00
	ATOM	11	N	MET A		6.663 -26.896	49.478 1.00 56.24
	MOTA	12	CA	MET A		6.435 -27.076	48.053 1.00 56.42
	ATOM	13	C	MET A		5.209 -26.282	47.619 1.00 56.07
40	ATOM	14	0	MET A			46.911 1.00 56.51
	ATOM	15	CB	MET A			47.788 1.00 60.46
	MOTA	16	CG	MET A		6.856 -29.020	46.477 0.00 99.00
	MOTA	17	SD	MET A		7.244 -30.775	46.483 0.00 99.00
4-	ATOM	18	CE	MET A		7.499 -30.975	44.711 0.00 99.00
45	ATOM	19	И	GLU A		4.035 -26.755	48.064, 1.00 54.92
	MOTA	20	CA	GLU A	. 2	2.803 -26.044	47.744 1.00 53.59

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	MOTA	16	CG	MET A	1	6.856 -29.020	46.477	0.00 99.00
	ATOM	17	SD	MET A	1	7.244 -30.775	46.483	0.00 99.00
	MOTA	18	CE	MET A	1	7.499 -30.975	44.711	0.00 99.00
	ATOM	19	N	GLU A	2	4.035 -26.755	48.064	1.00 54.92
5	MOTA	20	CA	GLU A	2	2.803 -26.044	47.744	1.00 53.59
-	ATOM	21	C	GLU A	2	2.870 -24.570	48.154	1.00 52.81
	ATOM	22	ō	GLU A	2	2.555 -23.664	47.393	1.00 51.69
	ATOM	23	CB	GLU A	2	1.661 -26.740	48.482	1.00 56.88
	ATOM	24	CG	GLU A	~ 2	2.090 -28.092	49.054	0.00 99.00
10	ATOM	25	CD	GLU A	2	1.019 -28.610	49.983	0.00 99.00
10	ATOM	26		GLU A	2	0.454 -27.819	50.722	0.00 99.00
		27		GLU A	2	0.761 -29.811	49.963	0.00 99.00
	ATOM	28		THR A	3	3.260 -24.346	49.424	1.00 52.06
	ATOM		N			3.300 -22.980	49.940	1.00 52.60
1.5	ATOM	29	CA	THR A	3	4.161 -22.059	49.070	1.00 50.30
15	MOTA	30	C	THR A	3		48.617	1.00 30.30
	ATOM	31	0	THR A	3	3.731 -21.006		
	MOTA	32	CB	THR A	3	3.858 -23.023	51.364	1.00 54.31
	MOTA	33	OG1		3	2.975 -23.789	52.187	1.00 56.98
~ ~	MOTA	34	CG2		3	3.960 -21.605	51.935	1.00 55.18
20	MOTA	35	N	LEU A	4	5.372 -22.498	48.717	1.00 50.11
	ATOM	36	CA	LEU A	4	6.201 -21.696	47.808	1.00 50.48
	MOTA	37	С	LEU A	4	5.553 - 21.516	46.444	1.00 50.18
	ATOM	38	0	LEU A	4	5.520 -20.410	45.877	1.00 50.73
	ATOM	39	CB	LEU A	4	7.603 -22.286	47.626	1.00 52.72
25	ATOM	40	CG	LEU A	4	8.545 -22.252	48.826	1.00 56.58
	ATOM	41	CD1	LEU A	4	9.819 -23.035	48.583	1.00 55.37
	ATOM	42	CD2	LEU A	4	8.829 -20.828	49.288	1.00 56.27
	MOTA	43	N	CYS A	5	5.028 -22.615	45.885	1.00 49.77
	ATOM	44	CA	CYS A	5	4.362 -22.530	44.587	1.00 48.93
30	ATOM	45	C	CYS A	5	3.218 -21.534	44.589	1.00 48.27
50	ATOM	46	ŏ	CYS A	5.	3.136 -20.698	43.682	1.00 47.03
	ATOM	47	СВ	CYS A	5	3.865 -23.879	44.075	1.00 49.50
	ATOM .		SG	CYS A	5	5.217 -24.972	43.626	1.00 50.79
		49	N	GLN A	6	2.356 -21.627	45.610	1.00 46.85
35	ATOM		CA	GLN A	6	1.227 -20.718	45.675	1.00 47.22
33	ATOM	50				1.666 -19.276	45.865	1.00 46.83
	MOTA	51	С	GLN A	6		45.276	1.00 40.65
	MOTA	52	0	GLN A	6	1.050 -18.382		
	MOTA	53	CB	GLN A	6	0.272 -21.079	46.817	1.00 50.54
40	MOTA	54	CG	GLN A	6	-0.681 -22.221	46.515	1.00 55.34
40	MOTA	55	CD	GLN A	6	-1.144 -22.875	47.806	1.00 59.63
	MOTA	56		GLN A	6	-1.101 -22.222	48.853	1.00 61.52
	MOTA	57	NE2	GLN A	6	-1.482 - 24.156	47.775	1.00 57.45
	ATOM	58	N	ARG A	7	2.628 -19.035	46.757	1.00 46.33
	MOTA	59	CA	ARG A	7	3.162 -17.700	46.938	1.00 46.38
45	MOTA	60	С	ARG A	7	3.780 -17.145	45.650	1.00 44.90
	ATOM	61	0	ARG A	7	3.544 -15.986	45.355	1.00 45.29
	ATOM	62	CB	ARG A	7	4.267 -17.682	48.013	1.00 50.84
	ATOM	63	CG	ARG A	7	3.690 -17.869	49.418	1.00 62.38
	ATOM	64	CD	ARG A	7	2.884 -16.616	49.765	1.00 71.41
50	ATOM	65	NE	ARG A	7	3.786 -15.539	50.171	1.00 78.82
	ATOM	66	CZ	ARG A	7	3.406 -14.307	50.474	1.00 83.50
	ATOM	67		ARG A	7	2.122 -13.965	50.423	1.00 85.24
	ATOM	68		ARG A	7	4.316 -13.410	50.841	1.00 85.59
	ATOM	69	N	LEU A	8	4.608 -17.918	44.984	1.00 45.22
55	MOTA	70	CA	LEU A	8	5.212 -17.429	43.728	1.00 45.85
55		71	CA	LEU A	. В	4.161 -17.110	42.672	1.00 46.67
	ATOM	72		LEU A	8	4.197 -16.055	42.025	1.00 46.25
	ATOM		O CD				43.194	1.00 40.23
	ATOM	73	CB	LEU A	8	6.185 -18.477		1.00 41.32
60	MOTA	74	CG	LEU A	8	6.979 -18.054	41.944	1.00 44.17
60	ATOM	75		LEU A	8	7.941 -16.924	42.283	
	MOTA	76		LEU A	8	7.723 -19.246	41.373	1.00 44.18
	ATOM	77	N	ASN A		3.193 -18.014	42.508	1.00 47.73
	ATOM	78	CA	ASN A	9	2:065 -17.825	41.610	1.00 48.73

	MOTA	79	С	ASN A	9	1.351 -16.516	41.925	1.00 48.98
	MOTA	80	0	ASN A	9	1.136 -15.727	40.999	1.00 48.98
	MOTA	81	CB	ASN A	9	1.011 -18.923	41.725	1.00 54.35
	ATOM	82	CG	ASN A	9	1.220 -20.167	40.912	1.00 58.01
5	ATOM	83		ASN A	9	2.281 -20.427	40.356	1.00 60.06
,	ATOM	84		ASN A	9	0.174 -20.991	40.841	1.00 63.02
	ATOM	85	N	VAL A	10	1.047 -16.267	43.206	1.00 48.31
	ATOM	86	CA	VAL A	10	0.388 -15.003	43.528	1.00 48.22
		87	C	VAL A	10	1.338 -13.837	43.252	1.00 48.34
10	ATOM		Ö	VAL A	10	0.931 -12.816	42.688	1.00 47.81
10	MOTA	88				-0.111 -14.918	44.981	1.00 53.07
	ATOM	89	CB	VAL A	10	-0.501 -13.487	45.353	1.00 53.07
	ATOM	90		VAL A	10			1.00 54.90
	ATOM	91		VAL A	10	-1.328 -15.827	45.176	
	ATOM	92	N	CYS A	11	2.601 -14.011	43.661	1.00 47.68
15	MOTA	93	CA	CYS A	11	3.570 -12.938	43.426	1.00 47.78
	MOTA	94	Ç	CYS A	11	3.747 -12.615	41.954	1.00 47.29
	ATOM	95	0	CYS A	11	3.632 -11.473	41.499	1.00 47.31
	ATOM	96	CB	CYS A	11	4.893 -13.269	44.144	1.00 48.13
	ATOM	97	SG	CYS A	11	6.077 -11.884	44.082	1.00 44.06
20	MOTA	98	N	GLN A	12	3.903 -13.633	41.120	1.00 47.63
	ATOM	99	CA	GLN A	12	4.150 -13.484	39.702	1.00 48.32
	ATOM	100	C	GLN A	12	2.936 -12.946	38.951	1.00 48.82
	ATOM	101	0	GLN A	12	3.103 -12.258	37.946	1.00 48.64
	ATOM	102	CB	GLN A	12	4.657 -14.783	39.092	1.00 45.97
25	ATOM	103	CG	GLN A	12	6.018 -15.213	39.590	1.00 45.90
	ATOM	104	CD	GLN A	12	6.659 -16.359	38.862	1.00 46.71
	ATOM	105		GLN A	12	6.028 -17.320	38.425	1.00 45.33
	ATOM	106		GLN A	12	7.983 -16.294	38.702	1.00 49.43
	MOTA	107	N	ASP A	13	1.736 -13.199	39.470	1.00 48.93
30	ATOM	108	CA	ASP A	13	0.516 -12.691	38.853	1.00 49.49
20	MOTA	109	C	ASP A	13	0.413 -11.198	39.085	1.00 49.55
	ATOM	110	ŏ	ASP A	13	0.082 -10.444	38.171	1.00 49.73
	ATOM	111	СB	ASP A	13	-0.732 -13.392	39.411	1.00 52.95
	ATOM	112	CG	ASP A	13	-0.955 -14.680	38.932	0.00 99.00
35	ATOM	113		ASP A	13	-0.110 -15.160	38.175	0.00 99.00
دد		114		ASP A	13	-2.054 -15.191	39.132	0.00 99.00
	ATOM					0.801 -10.735	40.269	1.00 48.95
	ATOM	115	И	LYS A	14	0.809 -9.313	40.556	1.00 49.25
	ATOM	116	CA	LYS A	14	1.794 -8.575	39.658	1.00 49.07
40	ATOM	117	C	LYS A	14		39.119	1.00 49.78
40	ATOM	118	0	LYS A	14	1.470 -7.519	42.030	1.00 49.78
	ATOM	119	CB	LYS A	14	1.109 -9.040		1.00 52.55
	ATOM	120	CG	LYS A	14	-0.070 -8.421	42.768	
	MOTA	121	CD	LYS A	14	-0.269 -6.975	42.329	1.00 66.42 1.00 70.58
4.5	ATOM	122	CE	LYS A	14	-1.227 -6.247	43.257	
45	ATOM	123	NZ	LYS A	14	-0.835 -4.824	43.452	1.00 72.01
	MOTA	124	N	ILE A	15	2.984 -9.131	39.468	1.00 48.82
	ATOM	125	CA	ILE A	15	3.992 -8.530	38.595	1.00 49.56
	MOTA	126	С	ILE A	15	3.467 -8.390	37.165	1.00 50.17
	ATOM	127	0	ILE A	15	3.538 -7.324	36.561	1.00 50.19
50	ATOM	128	CB	ILE A	15	5.288 -9.359	38.669	1.00 43.08
	ATOM	129	CG1	ILE A	15	5.931 -9.100	40.054	1.00 45.94
	ATOM	130	CG2	ILE A	15	6.286 -8.951	37.597	1.00 47.46
	ATOM	131	CD1	ILE A	15	6.960 -10.120	40.472	1.00 42.94
	MOTA	132	N	LEU A	16	2.880 -9.437	36.623	1.00 51.16
55	ATOM	133	CA	LEU A	16	2.272 -9.406	35.291	1.00 52.54
	ATOM	134	C	LEU A	16	1.135 -8.414	35.191	1.00 52.81
	ATOM	135	ŏ	LEU A	16	1.023 -7.678	34.194	1.00 53.37
	ATOM	136	СВ	LEU A	16	1.859 -10.810	34.847	1.00 56.20
	ATOM	137	CG	LEU A	16	3.067 -11.696	34.504	1.00 61.93
60	ATOM	138		LEU A	16	2.816 -13.139	34.904	1.00 65.17
00	ATOM	139		LEU A	16	3.456 -11.572	33.041	1.00 62.31
				THR A	17	0.274 -8.336	36.204	1.00 52.95
	ATOM ATOM	140 141	N CA	THR A	17	-0.789 -7.332	36.217	1.00 53.67
	AIUM	747	CM.	TUL W	1	0.103 -1.332	JU. ZI'	1.00 33.07

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	ATOM	142	С	THR	Α	17	-0.232	-5.916	36.173	1.00	54.28
	ATOM	143	ō	THR		17	-0.860	-5.026	35.590		54.21
	ATOM	144	СB	THR		17	-1.677	-7.468	37.468		55.51
	ATOM	145	OG1			17	-2.321	-8.742	37.469		54.73
5	ATOM	146	CG2			17	-2.713	-6.355	37.551		52.35
_	ATOM	147	N	HIS		18	0.879	-5.647	36.878		53.99
	ATOM	148	CA	HIS		18	1.495				
								-4.331	36.754		54.39
	ATOM	149	C	HIS		18	1.960	-4.115	35.313		55.01
10	ATOM	150	0	HIS		18	1.722	-3.036	34.757		54.91
10	ATOM	151	CB	HIS		18	2.663	-4.168	37.735		53.19
	MOTA	152	CG	HIS		18	2.198	-3.867	39.130		52.86
	ATOM	153		HIS		18	1.486	-2.733	39.432		52.60
	ATOM	154		HIS		18	2.362	-4.553	40.296		52.72
	ATOM	155	CE1	HIS	Α	18	1.216	-2.720	40.730	-1.00	53.99
15	ATOM	156	NE2	HIS	Α	18	1.735	-3.817	41.269	1.00	53.27
	MOTA	157	N	TYR	Α	19	2.580	-5.122	34.721	1.00	56.14
	MOTA	158	CA	TYR	Α	19	3.044	-5.034	33.337	1.00	58.17
	ATOM	159	С	TYR	Α	19	1.890	-4.733	32.380	1.00	58.92
	ATOM	160	0	TYR		19	1.957	-3.827	31.552		59.36
20	ATOM	161	CB	TYR		19	3.759	-6.320	32.950		59.47
	ATOM	162	CG	TYR		19	5.097	-6.621	33.580		62.05
	ATOM	163		TYR		19	5.983	-5.607	33.934		63.22
	ATOM	164	CD2			19	5.513	-7.934	33.787		62.96
	ATOM	165	CE1			19	7.212	~5.891	34.488		63.58
25	ATOM	166	CE2			19	6.745	-8.226	34.345		
23	ATOM	167	CZ				7.597				63.59
				TYR		19		-7.199	34.703		63.46
	ATOM	168	OH	TYR		19	8.828	-7.470	35.274		62.56
	ATOM	169	N	GLU		20	0.779	-5.451	32.499		59.63
20	ATOM	170	CA	GLU		20	-0.426	-5.196	31.734		59.76
30	ATOM	171	С	GLU		20	-0.990	-3.804	31.918		59.59
	ATOM	172	0	GLU		20	~1.198	-3.103	30.928		59.90
	ATOM	173	CB	GLU	A	20	-1.499	-6.241	32.056	1.00	66.29
	ATOM	174	CG	GLU	Α	20	-1.176	-7.583	31.409	1.00	73.88
	ATOM	175	CD	GLU	A	20	-2.142	-8.678	31.815	1.00	78.60
35	MOTA	176	OE1	GLU	Α	20	-1.749	-9.862	31.692	1.00	82.52
	ATOM	177	OE2	GLU .	Α	20	-3.272	-8.365	32.242	1.00	78.94
	ATOM	178	N	ASN .	Α	21	-1.186	-3.340	33.145		59.04
	ATOM	179	CA	ASN .	Α	21	-1.784	-2.053	33.404		57.97
	ATOM	180	С	ASN .		21	-1.002	-0.853	32.918		57.50
40	ATOM	181	0	ASN		21	-1.637	0.118	32.496		57.19
	ATOM	182	CB	ASN .		21	-2.149	-1.876	34.875		61.71
	ATOM	183	CG	ASN		21	-3.089	-2.964	35.362		63.07
	ATOM	184		ASN .		21	-3.691	-3.685			
	ATOM	185		ASN A		21			34.563		60.88
45	ATOM	186					-3.161	-3.066	36.685		62.59
7.0	ATOM		N	ASP A		22	0.327	-0.826	33.022		56.38
		187	CA	ASP A		22	1.080	0.299	32.480		54.54
	ATOM	188	C	ASP I		22	0.710	1.630	33.112		53.00
	ATOM	189	0	ASP I		22	0.632	2.652	32.424		52.65
50	ATOM	190	CB	ASP Z	•		0.818	0.005	50.50.		61.62
50	ATOM	191	CG	ASP A		22	2.107	0.655	30.214		65.99
	ATOM	192	OD1	ASP A	Ą	22	2.946	1.402	30.765	1.00	64.95
	ATOM	193	OD2	ASP A	Ą	22	2.235	0.116	29.099	1.00	69.58
	ATOM	194	N	SER A	A	23	0.616	1.683	34.440	1.00	50.98
	ATOM	195	CA	SER A	4	23	0.213	2.879	35.148	1.00	49.25
55	ATOM	196	С	SER A		23	1.294	3.960	35.095		48.02
	ATOM	197	ō	SER A		23	2.450	3.746	34.740		47.57
	ATOM	198	СВ	SER A		23	-0.101	2.633	36.640	1.00	
	ATOM	199	OG	SER A		23	0.549	1.424	36.984		56.16
	ATOM	200	N	THR A		24	0.847	5.152	35.441	1.00	
60	ATOM	201	CA	THR A		24	1.724	6.312	35.512		
	ATOM	202	C	THR A		24	1.724			1.00	
		202						6.860	36.920	1.00	
	ATOM		O	THR A		24	2.328	7.898	37.173	1.00	
	ATOM	204	CB	THR A	3	24	1.369	7.421	34.505	1.00	50.50

										•
	ATOM	205	OG1	THR A	24	`	0.042	7.871	34.734	1.00 51.02
	ATOM	206	CG2	THR A	24		1.558	6.901	33.094	1.00 48.60
	ATOM	207	N	ASP A	25		1.124	6.096	37.828	1.00 46.98
	MOTA	208	CA	ASP A	25		1.058	6.453	39.234	1.00 46.50
5	ATOM	209	С	ASP A	25		2.193	5.788	40.013	1.00 45.63
	ATOM .	210	0	ASP A	25		2.376	4.578	40.042	1.00 44.95
	ATOM	211	CB	ASP A	25	-	0.286	6.024	39.847	1.00 53.36
	ATOM	212	CG	ASP A	25		1.442	6.789	39.202	1.00 62.10
	ATOM	213	OD1	ASP A	25	_	1.605	7.997	39.498	1.00 64.72
10	ATOM	214	OD2	ASP A	25		2.185	6.192	38.392	1.00 62.72
	ATOM	215	N	LEU A	26		3.000	6.633	40.614	1.00 45.40
	MOTA	216	CA	LEU A	26		4.167	6.207	41.381	1.00 45.37
	MOTA	217	С	LEU A	26		3.834	5.157	42.418	1.00 45.85
	MOTA	218	0	LEU A	26	•	4.563	4.170	42.565	1.00 46.38
15	ATOM	219	CB	LEU A	26		4.763	7.483	41.982	1.00 44.87
	ATOM	220	CG	LEU A	26		6.056	7.341	42.783	1.00 44.69
	ATOM	221	CD1	LEU A	26		7.128	6.688	41.931	1.00 40.20
	MOTA	222	CD2	LEU A	26		6.529	8.703	43.267	1.00 46.93
	MOTA	223	N	ARG A	27		2.741	5.281	43.178	1.00 45.28
20	ATOM	224	CA	ARG A	27		2.266	4.241	44.065	1.00 45.19
	ATOM	225	С	ARG A	27		2.251	2.841	43.483	1.00 44.47
	ATOM	226	0	ARG A	27		2.610	1.886	44.187	1.00 44.56
	ATOM	227	CB	ARG A	27		0.852	4.494	44.607	1.00 51.04
	MOTA	228	CG	ARG A	27		0.713	5.531	45.690	1.00 61.27
25	ATOM	229	CD	ARG A	27		0.715	6.081	45.714	1.00 66.89
	MOTA	230	NE	ARG A	27		0.927	6.984	46.839	1.00 75.54
	ATOM	231	CZ	ARG A	27		2.083	7.555	47.170	1.00 79.36
	ATOM	232	NH1	ARG A	27		3.184	7.331	46.456	1.00 80.70
• •	ATOM	233	NH2	ARG A	27		2.152	8.359	48.228	1.00 79.78
30	ATOM	234	N	ASP A	28		1.771	2.632	42.255	1.00 43.06
	ATOM	235	CA	ASP A	28		1.785	1.318	41.648	1.00 41.77
	ATOM	236	С	ASP A	28		3.195	0.797	41.385	1.00 41.18
	MOTA	237	0	ASP A	28		3.408	-0.409	41.402	1.00 40.08
2.5	MOTA	238	CB	ASP A	28		1.014	1.325	40.303	1.00 44.91
35	MOTA	239	CG	ASP A	28		0.450	1.655	40.560	1.00 53.31
	ATOM	240		ASP A	28		1.014	2.560	39.920	1.00 53.29
	ATOM	241		ASP A	28		1.022	0.983	41.446	1.00 52.80
	ATOM	242	N	HIS A	29		4.132	1.700	41.062	1.00 40.87
40	ATOM	243	CA	HIS A	29		5.510	1.269	40.787	1.00 40.10
40	ATOM	244	С	HIS A	29		6.208	0.795	42.073	1.00 39.08
	ATOM	245	0	HIS A	29		6.987	-0.143	42.045	1.00 38.12
	MOTA	246	CB	HIS A	29		6.246	2.473	40.166	1.00 40.60
	MOTA	247	CG	HIS A	29		5.590	2.806	38.837	1.00 42.13
45	ATOM	248		HIS A	29		5.069	1.810	38.042	1.00 42.28
45	MOTA	249		HIS A	29		5.373	3.980	38.192	1.00 44.10
	MOTA	250		HIS A	29		1.552	2.348	36.943	1.00 43.73
	ATOM	251		HIS A	29		1.738	3.656	37.014	1.00 42.95
	ATOM	252	N	ILE A	30		5.896	1.454	43.152	1.00 39.44
50	ATOM	253	CA	ILE A			5.339		44.501	
50	ATOM	254	Ç	ILE A	30		5.899	-0.426	44.746	1.00 40.09
	ATOM	255	0_	ILE A	30		5.658	-1.303	45.181	1.00 41.16
	ATOM	256	CB	ILE A	30		5.843	1.991	45.550	1.00 40.65
	ATOM	257		ILE A	30		5.563	3.321	45.334	1.00 40.86
CE	ATOM	258		ILE A	30		5.125	1.537	47.004	1.00 41.39
55	ATOM	259		ILE A	30		5.060	4.498	46.138	1.00 42.24
	ATOM	260		ASP A	31		.631	-0.764	44.485	1.00 41.09
	ATOM .	261		ASP A	31		1.082	-2.089	44.758	1.00 40.37
	ATOM	262		ASP A	31		1.718	-3.130	43.856	1.00 40.59
60	ATOM	263		ASP A	31		1.965	-4.277	44.244	1.00 40.70
60	ATOM	264		ASP A	31		2.566	-2.080	44.459	1.00 42.53
	ATOM	265		ASP A	31		.886	-3.379	44.801	1.00 44.66
	ATOM	266		ASP A	31		.799	-4.311	43.991	1.00 46.03
	ATOM	267	OD2	ASP A	31	1	. 495	-3.517	45.987	1.00 53.28

	ATOM	268	N	TYR A	32	4.945	-2.735	42.589	1.00 39.00
	ATOM	269	CA	TYR A	32	5.636	-3.647	41.677	1.00 38.51
	ATOM	270	C	TYR A	32	7.017	-4.030	42.231	1.00 36.55
	ATOM	271	Ō	TYR A	32	7.359	-5.204	42.252	1.00 36.44
5	MOTA	272	CB	TYR A	32	5.765	-2.921	40.324	1.00 39.37
	ATOM	273	CG	TYR A	32	6.750	-3.532	39.369	1.00 42.61
	ATOM	274	CD1	TYR A	32	6.374	-4.668	38.646	1.00 45.04
	MOTA	275	CD2	TYR A	32	8.005	-2.989	39.141	1.00 43.12
10	MOTA	276	CE1	TYR A	32	7.245	-5.272	37.758	1.00 46.06
10	MOTA	277	CE2	TYR A	32 32	8.871 8.489	-3.576 -4.707	38.235 37.545	1.00 44.10 1.00 45.75
	MOTA MOTA	278 279	CZ OH	TYR A	32	9.322	-5.303	36.633	1.00 44.58
	ATOM	280	N	TRP A	33	7.850	-3.064	42.552	1.00 36.14
	ATOM	281	CA	TRP A	33	9.183	-3.384	43.061	1.00 36.59
15	ATOM	282	C	TRP A	33	9.144	-4.146	44.391	1.00 36.80
	ATOM	283	ō	TRP A	33	10.050	-4.951	44.634	1.00 37.42
	ATOM	284	CB	TRP A	33	10.054	-2.131	43.159	1.00 37.44
	MOTA	285	CG	TRP A	33	10.588	-1.813	41.780	1.00 34.77
	MOTA	286	CD1	TRP A	33	10.244	-0.745	40.979	1.00 35.47
20	ATOM	287	CD2	TRP A	33	11.522	-2.605	41.047	1.00 32.86
	ATOM	288	NE1	TRP A	33	10.974	-0.822	39.805	1.00 32.84
	MOTA	289	CE2	TRP A	33	11.735	-1.947 -3.792	39.799 41.301	1.00 35.43 1.00 32.38
	ATOM	290 291	CE3	TRP A	33 33	12.209 12.595	-2.444	38.832	1.00 32.38
25	ATOM ATOM	291	CZ3	TRP A	33	13.061	-4.282	40.337	1.00 33.33
23	ATOM	293	CH2	TRP A	33	13.245	-3.626	39.108	1.00 38.28
	ATOM	294	N	LYS A	34	8.150	-3.912	45.246	1.00 37.05
	ATOM	295	CA	LYS A	34	7.990	-4.765	46.437	1.00 37.56
	ATOM	296	С	LYS A	34	7.687	-6.205	46.060	1.00 37.90
30	MOTA	297	0	LYS A	34	8.220	-7.124	46.684	1.00 37.29
	MOTA	298	CB	LYS A	34	6.860	-4.261	47.345	1.00 36.29
	MOTA	299	CG	LYS A	34	7.111	-2.871	47.891	1.00 41.05
	MOTA	300	CD	LYS A	34	6.095	-2.498	48.945	1.00 47.20
25	ATOM	301	CE	LYS A	34	5.764	-1.032	48.964	1.00 49.66 1.00 57.26
35	ATOM	302	NZ	LYS A	34 35	5.046 6.853	-0.625 -6.411	50.219 45.025	1.00 37.20
	ATOM ATOM	303 304	N CA	HIS A	35	6.670	-7.779	44.525	1.00 37.30
	MOTA	305	C	HIS A	35	7.913	-8.328	43.875	1.00 35.96
	ATOM	306	Õ	HIS A	35	8.237	-9.523	43.986	1.00 34.61
40	ATOM	307	СВ	HIS A	35	5.446	-7.901	43.587	1.00 40.23
	ATOM	308	CG	HIS A	35	4.200	-7.883	44.428	1.00 44.09
	ATOM	309	ND1		35	3.567	-6.711	44.788	1.00 48.39
	ATOM	310	CD2	HIS A	35	3.539	-8.879	45.058	1.00 48.71
	MOTA	311		HIS A	35	2.538	-6.985	45.574	1.00 48.93
45	MOTA	312		HIS A	35	2.524	-8.283	45.774	1.00 47.98
	ATOM	313	N	MET A	36	8.665	-7.457	43.180	1.00 35.13
	ATOM	314	CA	MET A	36	9.927	-7.985	42.606 43.753	1.00 35.12 1.00 35.05
	ATOM	315	C	MET A MET A	36 36	10.836 11.472	-8.474 -9.504		1.00 33.03
50	MOTA MOTA	316 317	O CB	MET A	36	10.584	-6.890	41.772	1.00 34.78
50	ATOM	318	CG	MET A	36	9.832	-6.601	40.454	1.00 38.38
	ATOM	319	SD	MET A	36	10.026	-7.870	39.206	1.00 39.79
	ATOM	320	CE	MET A	36	11.681	-7.505	38.605	1.00 43.43
	MOTA	321	N	ARG A	37	10.903	-7.746	44.853	1.00 35.39
55	ATOM	322	CA	ARG A	37	11.729	-8.145	46.004	1.00 35.09
	ATOM	323	С	ARG A	37	11.240	-9.438	46.667	1.00 34.61
	MOTA	324	0	ARG A	37	12.028	-10.319	46.996	1.00 33.53
	ATOM	325	CB	ARG A	37	11.555	-7.001	47.018	1.00 34.72
CO	ATOM	326	CG	ARG A	37	12.370	-7.186	48.305	1.00 34.13
60	MOTA	327	CD	ARG A	37	12.132	-5.981	49.197	1.00 34.07
	ATOM	328	NE	ARG A	37	12.665	-6.189	50.551	1.00 35.48
	MOTA	329	CZ	ARG A	37	12.420	-5.313	51.520	1.00 33.64 1.00 38.49
	ATOM	330	MHT	ARG A	37	11.676	-4.228	51.375	1.00 30.49

	MOTA	331	NH2	ARG A	37	12.948 -5.572	52.719 1.	.00 32.86
	ATOM	332	N	LEU A	38	9.920 -9.544	46.841 1.	.00 33.92
	ATOM	333	CA	LEU A	38	9.330 -10.768	47.372 1.	.00 34.82
	ATOM	334	С	LEU A	38	9.592 -11.985	46.532 1.	.00 36.08
5	ATOM	335	ō	LEU A	38	9.879 -13.050	47.066 1.	.00 35.88
-	ATOM	336	СВ	LEU A	38	7.806 -10.549		.00 37.00
	ATOM	337	CG	LEU A	38	7.048 -11.843		00 39.41
	ATOM	338		LEU A	38	7.338 -12.303		00 36.17
					38	5.544 -11.698		00 42.91
10	ATOM	339		LEU A	39	9.532 -11.873		.00 36.01
10	ATOM	340	N	GLU A				.00 35.41
	ATOM	341	CA	GLU A	39	9.903 -12.982		
	ATOM	342	С	GLU A	39	11.310 -13.492		.00 35.95
	ATOM	343	0	GLU A	39	11.524 -14.706		.00 34.71
	ATOM	344	CB	GLU A	39	9.826 -12.621		.00 33.83
15	MOTA	345	CG	GLU A	39	9.999 -13.858		.00 35.55
	ATOM	346	CD	GLU A	39	10.153 -13.499		.00 44.56
	ATOM	347	OE1	GLU A	39	11.229 -12.997		.00 42.84
	ATOM	348	OE2	GLU A	39	9.219 -13.700	39.690 1.	.00 42.80
~	ATOM	349	N	CYS A	40	12.280 -12.600	44.916 1.	.00 35.37
20	ATOM	350	CA	CYS A	40	13.616 -13.054	45.262 1.	.00 35.02
	ATOM	351	С	CYS A	40	13.603 -13.852	46.574 1.	.00 35.78
	ATOM	352	Ō	CYS A	40	14.329 -14.842	46.621 1.	00 35.14
	ATOM	353	СВ	CYS A	40	14.587 -11.879		00 34.19
	ATOM	354	SG	CYS A	40	14.743 -10.845		00 35.07
25	ATOM	355	N	ALA A	41	12.796 -13.419		00 36.59
20	MOTA	356	CA	ALA A	41	12.772 -14.160		00 38.13
	ATOM	357	C	ALA A	41	12.191 -15.553		00 37.52
				ALA A	41	12.659 -16.527		00 38.32
	ATOM	358	0					00 36.08
20	ATOM	359	CB	ALA A	41	11.955 -13.380		00 37.54
30	MOTA	360	N	ILE A	42	11.221 -15.674	-	
	ATOM	361	CA	ILE A	42	10.629 -16.995		00 36.18
	ATOM	362	C	ILE A	42	11.626 -17.922		00 36.44
	MOTA	363	0	ILE A	42	11.856 -19.069		00 35.31
2.5	ATOM	364	CB	ILE A	42	9.325 -16.907		00 36.30
35	MOTA	365		ILE A	42	8.225 -16.165		00 38.51
	ATOM	366	CG2	ILE A	42	8.865 -18.282		.00 38.23
	MOTA	367	CD1	ILE A	42	7.114 -15.700		00 41.57
	MOTA	368	N	TYR A	43	12.321 -17.436		.00 35.53
	ATOM	369	CA	TYR A	43	13.341 -18.254	45.060 1.	00 36.20
40	MOTA	370	С	TYR A	43	14.479 -18.536		00 36.21
	ATOM	371	0	TYR A	43	15.091 -19.597	45.993 1.	00 36.69
	ATOM	372	CB	TYR A	43	13.884 -17.474	43.838 1.	00 36.61
	ATOM	373	CG	TYR A	43	13.065 -17.637	42.572 1.	00 38.55
	ATOM	374	CD1	TYR A	43	12.717 -16.512	41.820 1.	00 39.59
45	ATOM	375	CD2	TYR A	43	12.644 -18.871	42.116 1.	00 39.53
	ATOM	376		TYR A	43	11.998 -16.626		00 41.22
	ATOM	377	CE2	TYR A	43	11.943 -19.006		00 40.40
	ATOM	378	CZ	TYR A	43	11.604 -17.884		00 40.78
	ATOM	379	ОН		43	10.847 -17.954		00 41.19
50		380		TYR A	44	14.794 -17.563		00 35.43
30	ATOM		N CA			15.933 -17.815		00 37.45
	ATOM	381		TYR A	44			00 37.45
	ATOM	382	C	TYR A	44	15.547 -19.008		
	ATOM	383	0_	TYR A	44	16.329 -19.945		00 38.00
	ATOM	384	CB	TYR A	44	16.205 -16.555		00 38.20
55	ATOM	385	CG	TYR A	44	17.445 -16.670		00 40.09
	MOTA	386		TYR A	44	17.398 -17.286		00 41.30
	ATOM	387		TYR A	44	18.663 -16.206		00 40.77
	ATOM	388	CE1	TYR A	44	18.569 -17.412		00 42.23
	ATOM	389	CE2	TYR A	44	19.833 -16.312		00 42.80
60	ATOM	390	CZ	TYR A	44	19.746 -16.907		00 43.39
	ATOM	391	ОН	TYR A	44	20.863 -17.049	51.798 1.	00 45.51
	ATOM	392	N	LYS A	45	14.334 -18.982		00 38.11
	ATOM	393	CA	LYS A	45	13.891 -20.078		00 40.98
		-		·				

	MOTA	394	C	LYS A	45	13.832 -21.403 49.38	
	MOTA	395	0	LYS A	45 45	14.315 -22.472 49.78	
	ATOM ATOM	396 397	CB CG	LYS A LYS A	45	12.537 -19.754 50.75 11.968 -20.894 51.61	
5	ATOM	398	CD	LYS A	45	12.824 -21.269 52.81	
_	ATOM	399	CE	LYS A	45	12.671 -20.308 53.98	
	ATOM	400	NZ	LYS A	45	13.979 -20.145 54.69	
	ATOM	401	N	ALA A	46	13.307 -21.357 48.13	
	ATOM	402	CA	ALA A	46	13.230 -22.586 47.35	6 1.00 41.88
10	MOTA	403	С	ALA A	46	14.613 -23.167 47.17	9 1.00 41.96
	MOTA	404	0	ALA A	46	14.828 -24.368 47.34	7 1.00 42.06
	ATOM	405	CB	ALA A	46	12.561 -22.294 46.00	4 1.00 45.41
	ATOM	406	N	ARG A	47	15.605 -22.341 46.83	
• ~	ATOM	407	CA	ARG A	47	16.967 -22.806 46.64	
15	MOTA	408	C	ARG A	47	17.567 -23.364 47.94	
	MOTA	409	0	ARG A		18.270 -24.377 47.89	
	ATOM	410	CB	ARG A	47	17.873 -21.700 46.13	
	ATOM	411	CG	ARG A	47	19.278 -22.115 45.75	
20	ATOM	412	CD	ARG A	47	19.323 -23.087 44.56	
20	ATOM ATOM	413	NE	ARG A	47	20.701 -23.450 44.30	
	ATOM	414 415	CZ	ARG A ARG A	47	21.372 -24.042 43.35	
	ATOM	416		ARG A	47 47	20.819 -24.506 42.24 22.696 -24.175 43.51	
	ATOM	417	N.	GLU A	48	17.287 -22.673 49.05	
25	ATOM	418	CA.	GLU A	48	17.783 -23.090 50.36	
	ATOM	419	C	GLU A	48	17.266 -24.500 50.68	
	ATOM	420	ō	GLU A	48	18.009 -25.362 51.12	
	ATOM	421	СВ	GLU A	48	17.202 -22.208 51.47	
	ATOM	422	CG	GLU A	48	17.987 -21.039 51.95	
30	ATOM	423	CD	GLU A	48	17.911 -20.689 53.43	2 1.00 58.91
	ATOM	424	OE1	GLU A	48	16.891 -20.144 53.91	
	MOTA	425	OE2		48	18.904 -20.949 54.15	
	ATOM	426	N	MET A	49	16.000 -24.730 50.36	
35	ATOM	427	CA	MET A	49	15.358 -26.017 50.510	
33	ATOM ATOM	428 429	C O	MET A	49 49	15.738 -27.106 49.543 15.197 -28.218 49.620	
	ATOM	430	СВ	MET A	49	15.197 -28.218 49.626 13.840 -25.835 50.513	
	ATOM	431	CG	MET A	49	13.351 -25.048 51.719	
	ATOM	432	SD	MET A	49	11.617 -24.613 51.508	
40	ATOM	433	CE	MET A	49	10.922 -24.927 53.123	
	ATOM	434	N	GLY A	50	16.616 -26.852 48.593	
	ATOM	435	CA	GLY A	50	17.159 -27.787 47.664	
	MOTA	436	С	GLY A	50	16.332 -27.949 46.384	1.00 48.34
	ATOM	437	0	GLY A	50	16.603 -28.920 45.679	1.00 47.16
45	ATOM	438	N	PHE A	51	15.383 -27.074 46.084	
	ATOM	439	CA	PHE A	51	14.628 -27.205 44.83	
	ATOM	440	C	PHE A	51	15.442 -26.616 43.675	
	ATOM	441	0	PHE A	51	16.187 -25.659 43.884	
50	ATOM	442	CB	PHE A	51	13.266 -26.527 44.904	
50	ATOM ATOM	443 444	CG	PHE A	51 51	12.370 -27.030 46.005 12.237 -28.382 46.261	
	ATOM	445	CDI	PHE A	51	11.648 -26.142 46.784	
	ATOM	446		PHE A	51	11.418 -28.837 47.281	
	ATOM	447		PHE A	51	10.813 -26.584 47.788	
55	ATOM	448	CZ	PHE A	51	10.708 -27.937 48.047	
	ATOM	449	N	LYS A	52	15.455 -27.331 42.554	
	ATOM	450	CA	LYS A	52	16.204 -26.877 41.377	
	ATOM	451	C	LYS A	52	15.254 -26.192 40.393	
	ATOM	452	0	LYS A	52	15.644 -25.414 39.516	
60	ATOM	453	CB	LYS A	52	16.905 -28.073 40.739	
	ATOM	454	CG	LYS A	52	17.964 -28.697 41.640	
	ATOM	455	CD	LYS A	52	18.931 -29.536 40.811	
	ATOM	456	CE	LYS A	52	19.717 -30.537 41.711	0.00 99.00

	ATOM	457	NZ	LYS A	52		20.300 -31.674	41.001	0.00 99.00
	ATOM	458	N	HIS A	53		13.968 -26.480	40.589	1.00 46.17
	ATOM	459	CA	HIS A	53		12.924 -25.816	39.834	1.00 45.58
	ATOM	460	C	HIS A	53		11.697 -25.685	40.724	1.00 44.64
5	ATOM ·	461	0	HIS A	53		11.566 -26.465	41.649	1.00 44.95
	ATOM	462	CB	HIS A	53		12.568 -26.542	38.531	1.00 44.28
	ATOM	463	CG	HIS A	53		11.635 -27.700	38.758	1.00 46.45
	ATOM	464		HIS A	53		10.277 -27.525	38.978	1.00 45.21
1.0	ATOM	465		HIS A	53		11.868 -29.026	38.829	1.00 45.27
10	ATOM	466		HIS A	53		9.709 -28.698	39.163	1.00 45.18
	MOTA	467		HIS A	53		10.655 -29.629	39.076	1.00 49.44
	ATOM ATOM	468 469	N	ILE A	54 54		10.895 -24.693 9.598 -24.513	40.468	1.00 43.90
	ATOM	470	CA C	ILE A	54		8.589 -24.354	41.100 39.976	1.00 44.62 1.00 43.53
15	ATOM	471	ŏ	ILE A	54		8.704 -23.454	39.123	1.00 44.50
	ATOM	472	ČВ	ILE A	54		9.627 -23.258	41.996	1.00 51.01
	ATOM	473	CG1		54		8.222 -22.740	42.337	1.00 51.18
	ATOM	474	CG2		54		10.420 -22.138	41.313	1.00 54.51
	ATOM	475	CD1	ILE A	54		8.293 -22.022	43.690	1.00 55.08
20	MOTA	476	N	ASN A	55		7.679 -25.327	39.853	1.00 42.57
	ATOM	477	CA	ASN A	55		6.719 -25.332	38.748	1.00 41.98
	ATOM	478	С	ASN A	55		7.391 -25.383	37.389	1.00 41.70
	ATOM	479	0	ASN A	55		6.958 -24.848	36.368	1.00 41.10
25	ATOM	480	CB	ASN A	55		5.639 -24.266	38.828	1.00 41.18
25	ATOM	481	CG	ASN A	55		4.611 -24.596	39.915	1.00 45.37
	ATOM	482		ASN A	55		4.481 -25.766	40.285	1.00 42.95
	ATOM ATOM	483 484	ND2 N	ASN A HIS A	55 56		3.908 -23.589 8.508 -26.115	40.393 37.343	1.00 49.59
	ATOM	485	CA	HIS A	56		9.304 -26.336	36.155	1.00 42.09
30	ATOM	486	Ċ.	HIS A	56		9.996 -25.085	35.651	1.00 42.37
	ATOM	487	ō	HIS A	56		10.579 -25.115	34.573	1.00 41.39
	ATOM	488	CB	HIS A	56		8.509 -27.081	35.059	1.00 38.13
	ATOM	489	CG	HIS A	56	•	8.140 -28.417	35.639	1.00 39.93
	MOTA	490	ND1	HIS A	56		8.997 -29.476	35.683	1.00 40.64
35	MOTA	491		HIS A	56		7.000 -28.811	36.253	1.00 40.69
	ATOM	492		HIS A	56		8.401 -30.496	36.292	1.00 46.16
	ATOM	493		HIS A	56		7.192 -30.108	36.648	1.00 44.07
	MOTA	494	N	GLN A	57		10.115 -24.074	36.492	1.00 42.01
40	ATOM ATOM	495 496	CA C	GLN A GLN A	57 57		10.867 -22.845	36.209	1.00 43.31
40	ATOM	497	Ö	GLN A	5 <i>7</i>		12.178 -22.922 12.135 -23.367	37.011 38.159	1.00 42.73 1.00 42.65
	ATOM	498	СВ	GLN A	57		10.017 -21.730	36.771	1.00 44.03
	ATOM	499	CG	GLN A	57		10.191 -20.286	36.476	1.00 54.62
	ATOM	500	CD	GLN A	57		8.889 -19.530	36.723	1.00 54.38
45	ATOM	501	OE1	GLN A	57	,	8.881 -18.332	36.990	1.00 54.35
	ATOM	502	NE2	GLN A	57		7.774 -20.248	36.641	1.00 57.38
	ATOM	503	N	VAL A	58		13.308 -22.526	36.435	1.00 41.67
	ATOM	504	CA	VAL A	58		14.592 -22.695	37.122	1.00 41.06
50	ATOM	505	C	VAL A			14.654 -21.870		1.00 39.90
30	MOTA	506	0	VAL A	58		14.141 -20.751	38.425	1.00 40.26
	ATOM ATOM	507 508	CB CG1	VAL A VAL A	58 58		15.766 -22.343 15.770 -20.860	36.168 35.859	1.00 41.94
	ATOM	509		VAL A	58		17.085 -22.872	36.676	1.00 41.59 1.00 43.75
	ATOM	510	N	VAL A	59		15.193 -22.451	39.461	1.00 40.08
55	ATOM	511	CA	VAL A	59		15.414 -21.673	40.713	1.00 40.24
	ATOM	512	C	VAL A	59		16.878 -21.205	40.635	1.00 39.98
	ATOM	513	ō	VAL A	59		17.761 -22.042	40.559	1.00 41.27
	ATOM	514		VAL A	59		15.250 -22.591	41.945	1.00 40.48
	MOTA	515	CG1	VAL A	59		15.437 -21.777	43.243	1.00 44.12
60	MOTA	516		VAL A	59		13.830 -23.161	42.037	1.00 39.62
	ATOM	517	N	PRO A	60	_	17.121 -19.911	40.686	1.00 40.13
	ATOM	518		PRO A	60		18.466 -19.380	40.576	1.00 40.49
	ATOM	519	С	PRO A	60		19.312 -19.737	41.806	1.00 40.57

	ATOM	520	0	PRO	A	60	18.766 -20.039	42.863	1.00 39.38
	ATOM	521	СВ	PRO		60	18.272 -17.874	40.580	1.00 40.12
	MOTA	522	CG	PRO		60	16.837 -17.576	40.657	1.00 40.26
	ATOM	523	CD	PRO		60	16.069 -18.866	40.722	1.00 39.33
5	ATOM	524	N	THR		61	20.627 -19.662	41.632	1.00 39.59
5									1.00 39.51
	ATOM	525	CA	THR		61	21.502 -19.731	42.799	
	ATOM	526	C	THR		61	21.145 -18.651	43.803	1.00 38.37
	ATOM	527	0	THR		61	20.503 -17.621	43.545	1.00 37.40
	ATOM	528	CB	THR	A	61	23.000 -19.670	42.486	1.00 42.80
10	ATOM	529	OG1	THR	A	61	23.259 -18.498	41.695	1.00 42.80
	ATOM	530	CG2	THR	A	61	23.435 -20.914	41.722	1.00 42.91
	ATOM	531	N	LEU	Α	62	21.544 -18.931	45.058	1.00 37.77
	ATOM	532	CA	LEU		62	21.280 -17.966	46.132	1.00 36.91
	ATOM	533	C	LEU		62	21.841 -16.582	45.847	1.00 36.03
15	ATOM	534	ō	LEU		62	21.248 -15.566	46.209	1.00 36.36
10	MOTA	535	CB	LEU		62	21.904 -18.492	47.447	1.00 35.93
						62		47.950	1.00 35.33
	MOTA	536	CG	LEU			21.278 -19.807		
	MOTA	537		LEU		62	22.090 -20.339	49.139	1.00 44.24
00	ATOM	538		LEU		62	19.850 -19.557	48.450	1.00 33.58
20	ATOM	539	N	ALA		63	23.053 -16.511	45.336	1.00 36.59
	MOTA	540	CA	ALA	Α	63	23.729 - 15.236	45.091	1.00 36.90
	ATOM	541	С	ALA	Α	63	22.946 -14.476	44.014	1.00 36.28
	ATOM	542	0	ALA	Α	63	22.808 -13.263	44.128	1.00 35.61
	MOTA	543	CB	ALA		63	25.153 -15.402	44.601	1.00 39.35
25	ATOM	544	N	VAL		64	22.430 -15.198	43.013	1.00 35.11
	ATOM	545	CA	VAL		64	21.587 -14.456	42.054	1.00 35.89
	ATOM	546	C	VAL		64	20.370 -13.842	42.720	1.00 35.12
	ATOM	547	Õ	VAL		64	20.062 -12.664	42.487	1.00 34.59
20	ATOM	548	CB	VAL		64	21.180 -15.331	40.855	1.00 37.44
30	ATOM	549		VAL		64	20.071 -14.660	40.053	1.00 40.96
	ATOM	550		VAL		64	22.390 -15.680	40.014	1.00 36.95
	MOTA	551	N	SER	Α	65	19.616 -14.592	43.540	1.00 35.09
	MOTA	552	CA	SER	Α	65	18.477 -14.039	44.238	1.00 34.42
	ATOM	553	С	SER	Α	65	18.854 -12.961	45.225	1.00 34.48
35	ATOM	554	0	SER	Α	65	18.110 -11.986	45.326	1.00 34.19
	ATOM	555	CB	SER	Α	65	17.583 ~15.074	44.940	1.00 34.49
	ATOM	556	OG	SER	Α	65	17.165 -16.015	43.951	1.00 35.80
	ATOM	557	N	LYS		66	19.977 -13.079	45.922	1.00 34.79
	ATOM	558	CA	LYS		66	20.365 -11.976	46.828	1.00 35.44
40	ATOM	559	C	LYS		66	20.611 -10.670	46.044	1.00 35.50
	ATOM	560	ō	LYS		66	20.219 -9.590	46.478	1.00 35.28
	ATOM	561	СВ	LYS		66	21.709 -12.362	47.478	1.00 36.28
		562				66	21.492 -13.207	48.738	1.00 43.87
	ATOM		CG	LYS			22.772 -13.202	49.570	1.00 52.29
45	ATOM	563	CD	LYS		66			
43	ATOM	564	CE	LYS		66	23.722 -14.338	49.256	1.00 56.53
	ATOM	565	NZ	LYS		66	24.326 -14.857	50.541	1.00 60.41
	ATOM	566	N	ASN		67	21.345 -10.788	44.956	1.00 35.53
	ATOM	567	CA	ASN		67	21.679 -9.615	44.136	1.00 35.43
	MOTA	568	С	ASN	Α	67	20.452 -8.955	43.544	
50	ATOM	569	0	ASN	Α	67	20.370 -7.741	43.518	1.00 33.85
	ATOM	570	CB	ASN	Α	67	22.657 -10.003	43.019	1.00 39.24
	ATOM	571	CG	ASN	Α	67	22.999 -8.797	42.163	1.00 49.34
	ATOM	572		ASN		67	22.646 -8.711	40.977	1.00 55.32
	ATOM	573		ASN		67	23.611 -7.794	42.784	1.00 51.11
55	ATOM	574	N	LYS		68	19.505 -9.746	43.007	1.00 34.69
55								42.532	1.00 33.90
	ATOM	575 576	CA	LYS		68		42.532	1.00 33.50
	ATOM	576	C	LYS		68	17.421 -8.525		
,	ATOM	577	0	LYS		68	16.726 -7.530	43.412	1.00 32.16
60	ATOM	578	CB	LYS		68	17.439 -10.259	41.811	1.00 35.44
60	ATOM	579	CG	LYS		68	18.132 -10.664	40.503	1.00 38.74
	ATOM	580	CD	LYS		68	17.352 -11.710	39.729	1.00 44.24
	ATOM	581	CE	LYS		68	15.976 -11.178	39.345	1.00 46.97
	ATOM	582 -	NZ	LYS .	Α	68	15.414 -12.058	38.260	1.00 51.68

	ATOM	583	N	ALA A	A 69	17.395	-9.098	44.856	1.00 33.48
	ATOM	584	CA	ALA A	A 69	16.654	-8.440	45.924	1.00 33.17
	ATOM	585	С	ALA A		17.299	-7.103	46.282	1.00 31.99
	ATOM	586	ō	ALA A		16.620	-6.105	46.498	1.00 31.80
5	ATOM	587	ČВ	ALA A		16.642	-9.315	47.213	1.00 31.02
-	ATOM	588	N	LEU A		18.627	-7.019	46.312	1.00 32.54
	ATOM	589	CA	LEU A		19.278	-5.715	46.511	1.00 32.22
		590	C	LEU A		18.830	-4.668	45.471	1.00 32.04
	ATOM						-3.504	45.815	1.00 32.04
10	ATOM	591	0	LEU A		18.604			
10	ATOM	592	CB	LEU A		20.800	-5.876	46.425	1.00 35.34
	MOTA	593	CG	LEU A		21.431	-6.582	47.652	1.00 41.35
	ATOM	594		LEU A		22.952	-6.614	47.488	1.00 47.21
	MOTA	595		LEU A		21.124	-5.797	48.927	1.00 42.20
	MOTA	596	N	GLN A		18.732	-5.068	44.222	1.00 32.28
15	MOTA	597	CA	GLN A		18.336	-4.184	43.118	1.00 32.66
	ATOM	598	С	GLN A	A 71	16.888	-3.744	43.319	1.00 33.12
	ATOM	599	0	GLN A	A 71	16.599	-2.548	43.262	1.00 34.13
	ATOM	600	CB	GLN A	A 71	18.506	-4.847	41.767	1.00 32.48
	MOTA	601	CG	GLN A	A 71	19.933	-5.100	41.321	1.00 36.30
20	ATOM	602	CD	GLN A	71	20.143	-5.912	40.083	1.00 36.39
	ATOM	603		GLN A		21.103	-5.642	39.339	1.00 42.50
	ATOM	604		GLN A		19.349	-6.917	39.755	1.00 33.68
	ATOM	605	N	ALA A		16.008	-4.697	43.668	1.00 32.97
	ATOM	606	CA	ALA A		14.624	-4.358	43.963	1.00 32.73
25	ATOM	607	C	ALA A		14.529	-3.414	45.129	1.00 32.75
23						13.741	-2.468	45.153	1.00 33.02
	ATOM	608	0	ALA A					
	MOTA	609	СВ	ALA A		13.751	-5.597	44.164	1.00 31.63
	MOTA	610	N	ILE A		15.314	-3.700	46.205	1.00 32.96
20	MOTA	611	CA	ILE A		15.341	-2.754	47.321	1.00 32.98
30	ATOM	612	С	ILE A		15.756	-1.358	46.932	1.00 33.05
	MOTA	613	0	ILE A		15.173	-0.371	47.407	1.00 31.52
	ATOM	614	CB	ILE A		16.262	-3.309	48.450	1.00 32.37
	ATOM	615	CG1	ILE A	73	15.549	-4.497	49.099	1.00 34.48
	MOTA	616	CG2	ILE A	73	16.564	-2.217	49.479	1.00 36.05
35	ATOM	617	CD1	ILE A	73	16.442	-5.452	49.895	1.00 36.56
	ATOM	618	N	GLU A	74	16.821	-1.221	46.107	1.00 33.20
	ATOM	619	CA	GLU A		17.249	0.135	45.770	1.00 34.02
	ATOM	620	C	GLU A		16.127	0.888	45.042	1.00 33.88
	ATOM	621	ō	GLU A		15.924	2.077	45.333	1.00 33.58
40	ATOM	622	СВ	GLU F	_	18.483	0.128	44.849	1.00 42.88
	ATOM	623	CG	GLU A		19.730	-0.391	45.551	1.00 50.60
	ATOM	624	CD	GLU A		20.121	0.534	46.697	1.00 55.46
		625		GLU A		19.809	0.219	47.869	1.00 54.43
	ATOM				_			46.386	1.00 51.96
45	MOTA	626		GLU A		20.627	1.630 0.203		1.00 34.25
43	MOTA	627	N	LEU A		15.444		44.142	
	ATOM	628	CA	LEU A		14.353	0.814	43.393	1.00 34.85
	ATOM	629	С	LEU A		13.181	1.091	44.339	1.00 35.22
	MOTA	630	0	LEU A		12.683	2.215	44.292	1.00 35.32
~~	MOTA	631	CB	LEU A		13.895	-0.038	42.211	1.00 33.68
50	ATOM	632	CG	LEU A		14.632	0.175	40.849	1.00 40.28
	MOTA	633		LEU A		14.246	1.524	40.263	1.00 38.74
	ATOM	634	CD2	LEU A	75	16.134	0.148	41.044	1.00 41.33
	ATOM	635	N	GLN A	76	12.769	0.098	45.129	1.00 35.20
	ATOM	636	CA	GLN A	76	11.711	0.401	46.107	1.00 34.63
55	ATOM	637	C	GLN A		12.023	1.622	46.951	1.00 34.20
	ATOM	638	ŏ	GLN A		11.197	2.539	47.032	1.00 33.10
	ATOM	639	СВ	GLN A		11.439	-0.800	47.043	1.00 37.30
	ATOM	640	CG	GLN A		10.346	-0.570	48.086	1.00 36.76
	ATOM	641	CD	GLN A		10.511	-1.541	49.275	1.00 38.06
60	ATOM	642		GLN A		11.019	-2.647	49.273	1.00 36.12
J	ATOM						-1.178	50.481	1.00 30.12
		643 644		GLN A		10.136	1.702	47.596	1.00 34.42
	ATOM		N	LEU A		13.195			
	ATOM	645	CA	LEU A	. 77	13.533	2.857	48.402	1.00 34.29

	7.004		_		77	10 506			
	ATOM ATOM	646 647	C O	LEU A LEU A	77 77	13.506 13.070	4.183 5.221	47.638 48.149	1.00 34.87 1.00 32.77
	MOTA	648	СВ	LEU A	77	14.906	2.756	49.079	1.00 32.77
	ATOM	649	CG	LEU A	77	14.976	1.566	50.093	1.00 33.32
5	ATOM	650	CD:	l LEU A	77	16.417	1.466	50.566	1.00 35.24
	MOTA	651	CD2	2 LEU A	77	14.094	1.902	51.303	1.00 32.76
	MOTA	652	N	THR A	78	14.094	4.162	46.440	1.00 35.43
	ATOM	653	CA	THR A	78	14.147	5.391	45.644	1.00 35.16
10	ATOM	654	C	THR A	78	12.754	5.938	45.407	1.00 34.62
10	MOTA	655 656	0	THR A	78	12.561	7.128	45.655	1.00 35.48
	ATOM ATOM	657	CB OG1	THR A L THR A	78 78	14.869 16.212	5.117 4.853	44.306	1.00 33.75
	ATOM	658	CG2		78	14.710	6.309	44.644	1.00 36.55 1.00 35.96
	ATOM	659	N	LEU A	79	11.867	5.059	44.971	1.00 35.30
15	ATOM	660	CA	LEU A	79	10.492	5.458	44.646	1.00 35.23
	ATOM	661	С	LEU A	79	9.738	5.941	45.879	1.00 36.24
	ATOM	662	0	LEU A	79	8.923	6.848	45.814	1.00 34.44
	ATOM	663	CB	LEU A	79	9.744	4.326	43.961	1.00 37.56
	MOTA	664	CG	LEU A	79	10.302	3.825	42.611	1.00 40.81
20	ATOM	665		LEU A	79	9.415	2.708	42.066	1.00 36.86
	MOTA	666		LEU A	79	10.404	4.981	41.632	1.00 44.33
	MOTA	667	N	GLU A	80	10.058	5.284	47.023	1.00 35.96
	MOTA	668	CA	GLU A	80	9.487	5.773	48.285	1.00 35.25
. 25	ATOM ATOM	669 670	С 0	GLU A GLU A	80	10.002	7.132 7.941	48.672	1.00 35.81
. 23	ATOM	671	CB	GLU A	80 80	9.241 9.805	4.764	49.182 49.414	1.00 36.57 1.00 33.47
	ATOM	672	CG	GLU A	80 /		3.555	49.368	1.00 35.47
	ATOM	673	CD	GLU A	80	9.390	2.431	50.293	1.00 39.80
	ATOM	674	OE1		80	10.528	2.453	50.789	1.00 38.34
30	ATOM	675	OE2		80	8.587	1.482	50.397	1.00 40.54
	ATOM	676	N	THR A	81	11.266	7.474	48.443	1.00 35.85
	ATOM	677	CA	THR A	81	11.759	8.819	48.714	1.00 37.65
	ATOM	678	С	THR A	81	11.074	9.798	47.742	1.00 39.27
25	ATOM	679	0	THR A	81	10.711	10.894	48.159	1.00 38.93
35	ATOM	680	CB	THR A	81	13.277	8.895	48.523	1.00 38.88
	ATOM ATOM	681 682	OG1 CG2		81	13.854	8.188	49.626	1.00 41.45
	ATOM	683	N N	ILE A	81 82	13.827 10.887	10.315 9.360	48.511 46.500	1.00 37.76 1.00 39.69
	ATOM	684	CA	ILE A	82	10.176	10.260	45.568	1.00 39.09
40	ATOM	685	C	ILE A	82	8.727	10.458	45.979	1.00 42.17
	ATOM	686	Ö	ILE A	82	8.195	11.566	45.910	1.00 42.11
	ATOM	687	CB	ILE A	82	10.199	9.735	44.134	1.00 38.27
	MOTA	688	CG1	ILE A	82	11.619	9.500	43.651	1.00 39.22
4.0	MOTA	689	CG2		82	9.462	10.697	43.194	1.00 37.66
45	ATOM	690	CD1		82	12.489	10.717	43.731	1.00 43.59
	ATOM	691	N	TYR A	83	8.097	9.376	46.426	1.00 43.95
	ATOM	692	CA	TYR A	83	6.726	9.469	46.924	1.00 45.07
	ATOM ATOM	693 694	C O	TYR A TYR A	83 83	6.597	10.496	48.038	1.00 45.84
50	ATOM	695	СВ	TYR A	83	5.613 6.229	11.234 8.097	48.097 47.364	1.00 44.82 1.00 47.55
	ATOM	696	CG	TYR A	83	4.745	8.146	47.683	1.00 47.33
	ATOM	697		TYR A	83	3.826	8.070	46.643	1.00 53.71
	ATOM	698		TYR A	83	4.292	8.292	48.987	1.00 53.75
	ATOM	699		TYR A	83	2.469	8.119	46.899	1.00 55.59
55	MOTA	700	CE2	TYR A	83	2.932	8.343	49.245	1.00 55.42
	MOTA	701	CZ	TYR A	83	2.036	8.252	48.199	1.00 56.63
	MOTA	702	ОН	TYR A	83	0.691	8.313	48.454	1.00 58.49
	ATOM	703	N	ASN A	84	7.594	10.600	48.932	1.00 45.54
60	ATOM	704	CA	ASN A	84	7.519	11.621	49.959	1.00 46.22
	ATOM ATOM	705 706	C	ASN A	84 84	7.965 7.812	12.989	49.446	1.00 45.99
	ATOM	706	O CB	ASN A ASN A	84	7.812 8.199	13.930 11.252	50.226 51.257	1.00 46.80 1.00 45.97
	ATOM	708	CG	ASN A	84	7.995	9.970	52.011	1.00 43.97
							5.5.0	J J. I	1.00 32.27

	ATOM	709	Ωn	1 ASN A	84		6.960	9.292	51.955	1 00	48.67
	ATOM	710		2 ASN A			9.032				40.72
	ATOM	711	N	SER A			8.351		48.201		44.95
_	ATOM	712	CA				8.830	14.568	47.823		43.57
5	ATOM	713	C	SER A			7.800		46.988		43.08
	ATOM ATOM	714 715	O CB	SER A			6.747	14.845	46.627		41.05
	ATOM	716	OG	SER A SER A			10.108 9.782	14.456 14.024	46.969 45.656		43.41
	ATOM	717	N	GLN A	86		8.199	16.543	46.586		38.06 43.58
10	ATOM	718	CA	GLN A	86		7.377	17.394	45.725		44.93
	ATOM	719	C	GLN A	86		7.185	16.853	44.331		45.37
	ATOM	720	0	GLN A	86		6.311	17.326	43.581	1.00	45.62
	ATOM ATOM	721	CB	GLN A	86		8.100	18.761	45.588		52.00
15	ATOM	722 723	CG CD	GLN A GLN A	86 86		9.448	18.557	44.909		58.47
13	ATOM	724		GLN A	86		10.263 11.330	19.798 19.934	44.692 45.303		64.18 70.12
	ATOM	725	NE:		86		9.786	20.668	43.810		65.51
	MOTA	726	N	TYR A	87		8.002	15.875	43.915		45.13
20	ATOM	727	CA	TYR A	87		7.886	15.277	42.601		44.09
20	ATOM	728	C	TYR A	87		6.898	14.125	42.585		44.50
	ATOM ATOM	729 730	O	TYR A	87	•	6.682	13.536	41.536		43.83
	ATOM	731	CB CG	TYR A	87 87		9.231 10.318	14.748	42.072		42.80
	ATOM	732		L TYR A	87		11.376	15.782 15.539	42.226 43.084		41.15
25	ATOM	733		TYR A	87		10.272	17.010	41.567		39.57
	MOTA	734	CE	TYR A	87		12.344	16.496	43.319		41.24
	ATOM	735		YYR A	87		11.243	17.967	41.779		39.89
	ATOM	736	CZ	TYR A	87		12.295	17.693	42.614		40.85
30	ATOM ATOM	737 738	OH N	TYR A	87		13.302	18.594	42.842		41.44
50	ATOM	739	CA	SER A	88 88		6.318 5.478	13.805	43.743		45.60
	ATOM	740	C	SER A	88		4.368	12.626 12.534	43.844 42.814		46.49 47.16
	MOTA	741	ō	SER A	88		4.080	11.467	42.270		46.71
	ATOM	742	CB	SER A	88		4.816	12.633	45.245		48.13
35	ATOM	743	OG	SER A	88		4.092	11.417	45.346	1.00	51.98
	ATOM	744	N	ASN A	89		3.667	13.642	42.565		48.16
	ATOM ATOM	745 746	CA C	ASN A ASN A	89 89		2.563	13.593	41.604		49.94
	ATOM	747	o	ASN A	89		2.888 1.922	13.746 13.898	40.138 39.362		50.05 49.81
40	ATOM	748	ĊВ	ASN A	89		1.500	14.616	42.040		57.17
	ATOM	749	CG	ASN A	89		1.003	14.286	43.439		62.53
	ATOM	750		ASN A	89		0.752	15.195	44.234		67.35
	MOTA	751		ASN A	89		0.884	12.995	43.737		64.39
45	ATOM ATOM	752 753	N CA	GLU A	90		4.149	13.696	39.690		49.64
13	ATOM	754	CA	GLU A GLU A	90 90		4.384 3.952	13.669 12.346	38.238 37.610		49.09 48.60
	ATOM	755	ŏ	GLU A	90		3.715	11.386	38.327		47.76
	ATOM	756	CB	GLU A	90		5.891	13.782	37.891		47.16
	ATOM	757	CG	GLU A	90			14.906			42.61
50	ATOM	758	CD	GLU A	90		7.981	15.219	38.359	1.00	44.84
	ATOM	759		GLU A	90		8.767	14.356	37.961	1.00	
	ATOM ATOM	760 761	N N	GLU A LYS A	90 91		8.343	16.400	38.592	1.00	
	ATOM	762	CA	LYS A	91		3.961 3.798	12.276 10.985	36.269 35.595	1.00	
55	ATOM	763	c	LYS A	91		5.099	10.180	35.749	1.00	
	MOTA	764	Ō	LYS A	91		6.181	10.745	35.610	1.00	
	ATOM	765	CB	LYS A	91		3.615	11.124	34.076	1.00	48.52
	ATOM	766	CG	LYS A	91		2.234	10.887	33.509	1.00	55.86
60	ATOM	767	CD	LYS A	91		2.206	11.249	32.017	1.00	
00	ATOM ATOM	768 769	CE NZ	LYS A LYS A	91 91		2.934	10.173	31.214	1.00	
	ATOM	770	NZ N	TRP A	92		3.771 4.971	10.752 8.888	30.132 36.019	1.00	
	ATOM	771	CA	TRP A	92		6.082	7.961	36.101	1.00	
		_							-0.101	1.00	

	n mon	777		WDD 8							
	ATOM ATOM	772 773		TRP A			5.702				46.10
	ATOM	774		TRP A			4.701		35.668		
	ATOM	775					6.454		37.550		42.18
5	ATOM	776					6.876		38.372		37.28
	ATOM	777					6.025 8.170		39.126		35.98
	ATOM	778					6.703		38.526		35.45
	ATOM	779					8.031		39.704 39.359		37.68
	ATOM	780					9.436				34.31
10	ATOM	781					9.085		38.009 39.784		35.29
	ATOM	782					0.489		38.391		37.71 34.81
	ATOM	783					0.320	10.920	39.272		37.49
	ATOM	784	N	THR A			6.468	6.302	34.333		46.29
	ATOM	785					5.122	5.105	33.583		47.56
15	ATOM	786	C	THR A			5.901	3.910	34.110		48.41
	ATOM	787	Ō	THR A			7.846	4.126	34.862		48.37
	ATOM	788	CB				5.370	5.242	32.077		46.70
	MOTA	789	OG	1 THR A			7.740	4.928	31.792		44.41
	ATOM	790	CG				5.037	6.666	31.629		44.27
20	ATOM	791	N	LEU A			5.507	2.716	33.705		48.40
	ATOM	792	CA				.213	1.494	34.076	1.00	
	ATOM	793	C	LEU A			3.647	1.507	33.559		48.08
	MOTA	794	Ó	LEU A			587	1.053	34.225		47.67
	ATOM	795	СВ	LEU A			.462	0.294	33.479		56.38
25	ATOM	796	CG	LEU A	94		.488	-1.036	34.232		61.49
	ATOM	797	CD	1 LEU A	94		. 452	-0.872	35.741		61.80
	MOTA	798		2 LEU A	94		.310	-1.900	33.781		62.20
	ATOM	799	N	GLN A	95		.818	2.022	32.332		45.95
	ATOM	800	CA	GLN A	95		.175	2.149	31.805		43.86
30	ATOM	801	С	GLN A	95		.956	3.201	32.555		41.09
	ATOM	802	0	GLN A	95		.138	2.966	32.803		42.10
	ATOM	803	CB	GLN A	95		.226	2.431	30.291		47.51
	ATOM	804	CG	GLN A	95		.933	1.311	29.532		55.82
	ATOM	805	CD	GLN A	95		.441	1.369	29.531		58.57
35	ATOM	806	OE:	l GLN A	95	13	.085	2.191	28.850		63.35
	MOTA	807	NE:	2 GLN A	95	13	.089	0.470	30.270		53.71
	ATOM	808	N	ASP A	96	10	.358	4.296	32.984		39.88
	ATOM	809	CA	ASP A	96	11	.048	5.272	33.814		39.85
40	ATOM	810	С	ASP A	96	11	.651	4.615	35.076	1.00	40.22
40	ATOM	811	0	ASP A	96	12	.731	5.042	35.499	1.00	39.43
	ATOM	812	CB	ASP A	96	10	.115	6.397	34.246	1.00	40.26
	ATOM	813	CG	ASP A	96	9	.603	7.287	33.110	1.00	43.09
	ATOM	814	OD1		96		.290	7.391	32.079	1.00	38.82
15	ATOM	815		ASP A	96		.516	7.883	33.274	1.00	41.58
45	MOTA	816	N	VAL A	97		.956	3.643	35.651	1.00	39.44
	ATOM	817	CA	VAL A	97		.371	3.024	36.913	1.00	38.84
	ATOM	818	С	VAL A	97		.979	1.641	36.744	1.00	38.61
	ATOM	819	0	VAL A	97		.059	0.843	37.707		38.87
50	ATOM	820	CB	VAL A	97		.186	2.955	37.903		40.58
50	MOTA	821		VAL A	97		.561	4.325	38.123		37.24
	ATOM	822		VAL A	97		.122	1.929	37.569		39.40
	ATOM	823	N	SER A	98		. 431	1.314	35.539		37.55
,	ATOM	824	CA	SER A	98 .		. 956	0.014	35.183		36.27
55	ATOM	825	C	SER A	98		. 408	-0.046	35.652	1.00	36.46
در	ATOM	826	0	SER A	98		.028	1.015	35.744		36.95
	ATOM	827	CB	SER A	98		915	-0.142	33.637		41.66
	ATOM	828	OG	SER A	98		869	0.716	32.996	1.00	
	ATOM	829	N	LEU A	99		941	-1.247	35.831	1.00	
60	ATOM ATOM	830	CA	LEU A	99		345	-1.378	36.203	1.00	
00	ATOM	831 832	С 0	LEU A LEU A	99		251	-0.939	35.042	1.00	
	ATOM	833	СВ	LEU A	99 99		297	-0.341	35.258	1.00	
	ATOM	834	ÇG	LEU A	99		636	-2.829	36.589	1.00	
	.11011	0.34	Ų.G	TEC W	23	19.	056	-3.111	37.080	1.00	45.46

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	ATOM	835	CD1	LEU .	A 99	18.330	-2.481	38.442	1.00	43.84
	ATOM	836	CD2	LEU .	A 99	18.341		37.072		45.55
	ATOM	837	N	GLU I	A 100	16.797		33.818	1.00	36.41
	ATOM	838	CA	GLU	A 100	17.488		32.611		37.21
5	ATOM	B39	C		A 100	17.790		32.622		36.02
-	ATOM	840	ŏ		A 100	18.972		32.470		37.81
	ATOM	841	СВ		A 100	16.690		31.340		
	ATOM	842	CG		A 100	17.528				40.11
	ATOM	843	CD					30.096		49.41
10	ATOM	844			A 100	16.866		28.790		56.89
10	ATOM			GLU A		15.724	-1.755	28.761		57.99
		845		GLU A		17.534	-1.025	27.753		62.25
	ATOM	846	N		A 101	 	1.580	32.792		35.41
	ATOM	847	CA		A 101	17.044	3.010	32.973		34.54
1.5	ATOM	848	C		1 101	17.897	3.329	34.185	1.00	34.62
15	ATOM	849	0		101	18.899	4.082	34.151	1.00	33.43
	ATOM	850	CB		101	15.666	3.714	33.047	1.00	36.71
	ATOM	851	CG1	VAL A	101	15.797	5.167	33.459	1.00	34.93
	ATOM	852	CG2	VAL A	101	15.013	3.600	31.651	1.00	37.61
	MOTA	853	N	TYR A	102	17.555	2.678	35.314	1.00	33.28
20	MOTA	854	CA	TYR A	102	18.202	3.008	36.583		33.58
	ATOM	855	С	TYR A	102	19.711	2.817	36.484		33.46
	MOTA	856	0	TYR A		20.424	3.624	37.071		33.95
	ATOM	857	ČВ	TYR A		17.653	2.091	37.691		34.23
	ATOM	858	CG	TYR A		17.996	2.494	39.103		36.50
25	ATOM	859	CD1			17.325	3.559	39.676		
	ATOM	860	CD2			18.961				36.36
	ATOM	861	CE1	TYR A			1.811	39.855		36.63
	ATOM	862				17.582	3.949	40.979		37.25
				TYR A		19.237	2.202	41.162		37.64
30	ATOM	863	CZ	TYR A		18.537	3.253	41.707		36.95
30	ATOM	864	ОН	TYR A		18.795	3.693	42.966		36.81
	ATOM	865	N	LEU A		20.170	1.800	35.766	1.00	32.90
	ATOM	866	CA	LEU A		21.575	1.513	35.625		34.69
	MOTA	867	С	LEU A		22.225	2.188	34.422	1.00	35.97
2.0	ATOM	868	0	LEU A		23.434	2.037	34.247	1.00	37.11
35	ATOM	869	CB	LEU A		21.811	0.003	35.568	1.00	34.47
	MOTA	870	CG	LEU A	103	21.363	-0.757	36.853	1.00	39.98
	ATOM	871	CD1	LEU A	103	21.588	-2.261	36.702	1.00	40.37
	MOTA	872	CD2	LEU A	103	22.104	-0.231	38.073		40.86
	ATOM	873	N	THR A	104	21.460	2.913	33.614		35.72
40	ATOM	874	CA	THR A		22.115	3.606	32.468		34.87
	ATOM	875	С	THR A		22.792	4.825	33.060		35.15
	ATOM	876	0	THR A		22.206	5.345	34.004		35.03
	ATOM	877	СB	THR A		21.074	4.013	31.409		36.04
	ATOM	878	OG1	THR A		20.507	2.790	30.928		34.78
45	ATOM	879		THR A		21.709	4.722	30.211		
	ATOM	880		ALA A		23.907	5.292			36.74
	ATOM	881						32.541		35.32
	ATOM	882		ALA A		24.595	6.446	33.150		36.34
	ATOM			ALA A		23.662	7.647	33.117		36.12
50				ALA A		23.031				35.49
50	ATOM			ALA A		25.840	6.710	32.281		36.09
	ATOM		N	PRO A		23.556	8.404	34.195		35.90
^	ATOM			PRO A	106	24.273	8.154	35.428	1.00	36.06
	ATOM	887	С	PRO A	106	23.617	7.057	36.275	1.00	35.41
	ATOM	888	0	PRO A	106	22.426	7.141	36.602		34.13
55	MOTA	889	CB	PRO A	106	24.167	9.484	36.175		36.61
	MOTA	890		PRO A		22.880	10.077	35.695		36.41
	ATOM			PRO A		22.862	9.725	34.223		36.94
	ATOM			THR A		24.407	6.045	36.646		35.50
	ATOM			THR A		23.833	4.857	37.287		34.62
60	ATOM			THR A		23.256	5.142	38.651		34.62
	ATOM			THR A		23.236				
	ATOM			THR A			6.108	39.324		34.98
	ATOM					24.820	3.666	37.301	1.00	
	AIOM	897	OGI ,	THR A	10/	24.114	2.516	37.812	1.00	36.86

5	ATOM MOTA MOTA MOTA MOTA MOTA MOTA	898 899 900 901 902 903 904 905	CG2 N CA C O N CA C	GLY GLY GLY CYS CYS	A 107 A 108 A 108 A 108 A 108 A 109 A 109 A 109	26.016 22.272 21.709 20.719 20.469 20.099 19.226 17.997	3.957 4.352 4.504 5.660 6.140 6.080 7.257 6.934	38.203 39.091 40.436 40.527 41.6427 39.427 39.416 38.551		5.80 5.25 5.77 5.22 4.86 5.48
10	ATOM ATOM ATOM	906 907 908	O CB SG	CYS	A 109 A 109 A 109	18.179 19.987 21.181	6.397 8.395 9.249	37.449 38.610 39.651	1.00 3 1.00 3 1.00 4	6.31 5.03
	MOTA MOTA MOTA	909 910 911	N CA C	ILE	A 110 A 110 A 110	16.785 15.613 15.774	7.158 7.181 8.456	39.035 38.156 37.264	1.00 3 1.00 3	4.76
15	ATOM ATOM	912 913	O CB	ILE	A 110 A 110	16.234 14.315	9.494 7.414	37.723 38.954	1.00 3 1.00 3	2.60 7.69
20	ATOM ATOM ATOM ATOM ATOM ATOM	914 915 916 917 918 919	CG2 CD1 N CA C	ILE ILE LYS LYS LYS	A 110 A 110 A 110 A 111 A 111 A 111	14.117 13.100 13.770 15.373 15.522 14.453	6.274 7.594 4.943 8.287 9.400 9.355	39.951 38.049 39.384 36.013 35.086 34.002	1.00 43 1.00 33 1.00 43 1.00 33 1.00 35	9.85 3.84 1.15 5.30
25	ATOM ATOM ATOM	920 921 922	O CB CG	LYS .	A 111 A 111 A 111	13.942 16.879 17.713	8.285 9.488 8.300	33.702 34.449 34.171	1.00 35 1.00 35 1.00 44	9.11
	ATOM ATOM ATOM	923 924 925	CD CE NZ	LYS .	A 111 A 111 A 111	19.195 19.930 19.943	8.574 7.270 6.341	34.494 34.207 35.377	1.00 41 1.00 41 1.00 36	.21
30	ATOM ATOM ATOM ATOM	926 927 928 929	N CA C O	LYS I	A 112 A 112 A 112 A 112	14.181 13.194 13.553 14.382	10.569 10.511 11.477	33.482 32.410 31.283 31.442	1.00 36 1.00 37 1.00 38	1.12
35	ATOM ATOM ATOM	930 931 932	CB CG CD	LYS Z	A 112 A 112 A 112	11.784 11.274 9.855	12.368 10.464 11.108	32.883 34.092	1.00 37 1.00 45 1.00 43	.17
25	ATOM ATOM	933 934	CE NZ	LYS A	A 112 A 112	9.625 8.251	10.826 11.830 12.207	34.592 35.702 36.085	1.00 42 1.00 40 1.00 41	.92
40	ATOM ATOM ATOM ATOM ATOM	935 936 937 938 939	CA C O CB	HIS A HIS A HIS A		12.734 12.848 14.221 14.895 12.341	11.353 12.198 12.110 13.102 13.611	30.256 29.053 28.430 28.197 29.366	1.00 38 1.00 39 1.00 40 1.00 38	.66 .88 .77
45	ATOM ATOM ATOM ATOM ATOM	940 941 942 943 944	ND1 CD2 CE1	HIS A HIS A HIS A HIS A	113 113 113	11.036 9.924 10.680 8.934 9.378	13.636 12.958 14.172 13.113 13.838	30.115 29.655 31.299 30.518 31.529	1.00 38 1.00 42 1.00 41 1.00 37 1.00 43	.21 .13 .50
50	ATOM ATOM ATOM	945 946 947 948	CA C O	GLY A GLY A GLY A GLY A	114 114 114	14.678 15.948 15.982 15.006	10.906 10.634 10.869 10.756	28.098 27.465 25.944 25.196	1.00 40 1.00 42 1.00 42 1.00 43	.07 .05
55	ATOM ATOM ATOM ATOM ATOM	949 950 951 952 953	CA C	TYR A TYR A TYR A TYR A	115 115 115	17.172 17.369 18.822 19.673 17.029	11.210 11.441 11.155 11.182 12.863	25.445 24.019 23.637 24.526 23.612	1.00 42 1.00 42 1.00 42 1.00 40 1.00 43	.59 .83 .37
60	ATOM ATOM ATOM ATOM ATOM ATOM ATOM	954 955 956 957 958 959	CG CD1 CD2 CE1 CE2 CZ	TYR A	115 115 115 115 115	17.877 18.944 17.628 19.718 18.375 19.398 20.194	13.912 14.514 14.263 15.463 15.230 15.845 16.754	24.298 23.648 25.614 24.291 26.260 25.579 26.228	1.00 45 1.00 47 1.00 47 1.00 47 1.00 47 1.00 48 1.00 49	.80 .34 .05 .70 .78

	MOTA MOTA MOTA	961 962 963	CA	THR	A 1: A 1: A 1:	16	19.071 20.415 21.285	10.564	21.938	1.00	41.33 42.28 42.08
5	ATOM ATOM ATOM	964 965 966	O CB OG1	THR THR		6	20.858 20.365 19.589	12.791 9.722 8.542	21.136 20.643 20.949	1.00 1.00 1.00	42.54 46.87 49.86
10	ATOM ATOM ATOM ATOM	967 968 969 970	CG2 N CA C	VAL VAL VAL	A 11 A 11	7	21.753 22.552 23.575 24.538		20.209 22.045 21.686 20.830	1.00	46.71 40.95 40.83 41.40
	ATOM ATOM ATOM	971 972 973	O CB CG1	VAL VAL VAL	A 11 A 11 A 11	.7 .7 .7 _.	24.850 24.297 25.599	10.689	21.222 22.928 22.569	1.00 1.00	41.22 39.95 41.09
15	ATOM ATOM ATOM ATOM	974 975 976 977	CG2 N CA C	VAL GLU GLU GLU	A 11 A 11	.8 .8	23.375 24.986 25.908 27.254	14.216 12.396 11.573 12.265	23.617 19.713 18.905	1.00 1.00	38.93 41.76 42.29
20	MOTA MOTA MOTA	978 979 980 981	O CB CG CD	GLU GLU GLU	A 11 A 11 A 11 A 11	8 8 8	27.288 25.266 25.923 25.542	13.498 11.262 11.896 11.270	18.832 18.801 17.556 16.365 15.029	1.00 1.00 1.00	42.60 42.94 46.34 53.27 55.37
25	ATOM ATOM ATOM ATOM ATOM	982 983 984 985 986		GLU GLU VAL VAL VAL	A 11 A 11 A 11	8 9 9	24.442 26.425 28.322 29.661 30.408	10.707 11.358 11.485 12.031 11.363	14.879 14.155 18.947 18.909 17.735	1.00 1.00 1.00	54.40 57.58 41.77 42.33
20	ATOM ATOM ATOM	987 988 989	O CB CG1	VAL . VAL .	A 11 A 11 A 11	9 9 9	30.499 30.486 31.894	10.136 11.790 12.330	17.672 20.187 19.963	1.00 1.00 1.00	43.93 42.59 42.91 40.51
30	ATOM ATOM ATOM	990 991 992 993	N CA C	GLN GLN GLN	A 12 A 12 A 12	0 0 0	29.868 30.927 31.698 33.182	12.517 12.212 11.727 11.912	21.398 16.870 15.723 16.001	1.00 1.00 1.00	38.33 44.65 47.49 50.11
35	ATOM ATOM ATOM ATOM	994 995 996 997	O CB CG CD	GLN Z GLN Z GLN Z	A 12 A 12	D D	33.676 31.330 29.834 29.456	13.040 12.541 12.547 13.089	16.117 14.481 14.248 12.884	1.00	48.28 48.85 52.37 55.34
40	ATOM ATOM ATOM ATOM ATOM	998 999 1000 1001 1002		GLN A GLN A PHE A PHE A	A 120 A 120 A 120	0 1 1	30.319 28.164 33.872 35.287 36.147	13.536 13.016 10.771 10.824 11.092	12.135 12.580 16.065 16.382 15.162	1.00 1.00 1.00 1.00	59.08 56.41 52.87 58.51 62.63
45	ATOM ATOM ATOM ATOM ATOM	1003 1004 1005 1006 1007	O CB CG CD1	PHE PHE PHE PHE PHE PHE	12: 12: 12: 12: 12:	L L L	37.367 35.764 35.110 33.983	11.134 9.660 9.596 8.822	15.318 17.219 18.571 18.763	1.00 1.00 1.00 1.00	63.15 54.96 55.06 54.70
50	ATOM ATOM ATOM ATOM	1008 1009 1010 1011	CE1 CE2 CZ N	PHE F PHE F PHE F ASP F	121 121 121 122	L L	35.627 33.389 35.032 33.908 35.547	10.295 8.726 10.209 9.438 11.249	19.641 20.000 20.885 21.065 13.988	1.00 1.00 1.00	52.63 54.52 53.27 53.03 66.78
55	ATOM ATOM ATOM ATOM	1012 1013 1014 1015	С 0	ASP A ASP A ASP A	122	<u> </u>	36.246 35.414 35.591 37.480	11.801 12.152 13.228 10.970	12.847 11.632 11.042 12.495	1.00 1.00 1.00	72.12 74.59 75.06 80.67
	ATOM ATOM ATOM	1016 1017 1018	CG OD1 OD2	ASP A ASP A ASP A	122 122 122		38.640 38.366 39.782	11.910 13.018 11.512	12.201 11.687 12.508	1.00 1.00 1.00	84.98 87.13 89.25
60	ATOM ATOM ATOM ATOM ATOM	1019 1020 1021 1022 1023	CA C O	GLY A GLY A GLY A GLY A ASP A	123 123 123		34.511 33.653 32.499 32.702 31.278	11.277 11.544 10.546 9.332 11.063	11.204 10.050 9.975 10.039 9.813	1.00 1.00 1.00 1.00	79.12 80.59 80.64

	ATOM ATOM ATOM	1024 1025 1026	CA C O	ASP	A 12 A 12 A 12	4 30.000	10.180 9.574 9.777	9.717 8.324 7.400	1.00 82.77 1.00 82.74 0.00 99.00
5	MOTA MOTA	1027 1028	CB CG		A 12	4 28.828	10.863	10.141	1.00 87.39
	ATOM	1029	OD1	ASP	A 12	4 28.495	8.933	11.489	1.00 93:18
	ATOM	1030	OD2				10.288	11.244	1.00 93.68
	MOTA	1031	N	ASN			6.401	13.268	1.00 58.22
10	ATOM ATOM	1032 1033	CA C	ASN ASN			5.964 6.983	14.601 15.144	1.00 58.81 1.00 58.26
	ATOM	1034	Ö	ASN .			8.096	15.144	1.00 58.82
	ATOM	1035	ČВ	ASN			5.955	15.579	1.00 58.33
	MOTA	1036	CG	ASN .	A 127	7 35.959	4.889	15.347	1.00 62.63
1.5	MOTA	1037	OD1				3.697	15.490	1.00 64.16
15	ATOM	1038	ND2				5.307	15.008	1.00 60.87
	ATOM	1039	N	THR .			6.617	15.180	1.00 57.71
	ATOM ATOM	1040 1041	CA C	THR I			7.522 6.846	15.665 16.795	1.00 57.23 1.00 56.48
	MOTA	1041	Ö	THR			5.792	16.793	1.00 56.48
20	ATOM	1043	CB	THR			7.842	14.501	1.00 56.65
	ATOM	1044	OG1				8.579	13.536	1.00 57.99
	MOTA	1045	CG2	THR I	A 128		8.653	14.901	1.00 56.34
	MOTA	1046	N	MET A			7.406	18.002	1.00 54.99
25	MOTA	1047	CA	MET I			6.817	19.175	1.00 52.19
25	ATOM	1048	C	MET I			7.511	19.533	1.00 50.42
	ATOM ATOM	1049 1050	O CB	MET A	A 125		8.705 6.909	19.319 20.391	1.00 48.93 1.00 58.00
	ATOM	1051	CG	MET A			5.934	20.458	1.00 58.00
	ATOM	1052	SD	MET A			4.263	20.904	1.00 68.26
30	ATOM	1053	CE	MET A			4.518	22.510	1.00 68.01
	ATOM	1054	N	HIS A			6.735	20.126	1.00 49.01
	MOTA	1055	CA	HIS A			7.194	20.571	1.00 47.13
		_1056	С	HIS A			7.057	22.095	1.00 46.21
35	ATOM ATOM	1057 1058	O CB	HIS A			6.118 6.345	22.678 19.956	1.00 45.61
55	ATOM	1059	CG	HIS A			6.751	18.602	1.00 53.82 1.00 62.48
	ATOM	1060		HIS A			7.119	17.581	1.00 66.97
	MOTA	1061	CD2	HIS A	130		6.825	18.084	1.00 65.45
40	ATOM	1062		HIS A			7.424	16.505	1.00 67.80
40	ATOM	1063		HIS A			7.252	16.784	1.00 68.13
	MOTA	1064	N	TYR A			8.097	22.775	1.00 43.95
	ATOM ATOM	1065 1066	CA C	TYR F			8.130 8.666	24.227 24.576	1.00 42.51 1.00 41.94
	ATOM	1067	ŏ	TYR F			9.497	23.829	1.00 41.94
45	ATOM	1068	СВ	TYR A			9.151	24.762	1.00 42.89
	ATOM	1069	CG	TYR A			8.830	24.392	1.00 42.97
	MOTA	1070	CD1	TYR A	131		9.421	23.240	1.00 42.76
	MOTA	1071		TYR A			7.993	25.131	1.00 43.24
50	ATOM	1072		TYR A			9.187	22.828	1.00 44.91
30	ATOM ATOM	1073		TYR A			7.765	24.728	1.00 45.47
	ATOM	1074 1075	CZ OH	TYR A		29.991 31.295	8.365 8.087	23.587 23.222	1.00 46.72 1.00 49.71
	ATOM	1076	N	THR A			8.297	25.721	1.00 49.71
	ATOM	1077		THR A		21.666	8.825	26.098	1.00 37.97
55	ATOM	1078		THR A		21.835	9.967	27.066	1.00 37.49
	ATOM	1079	0	THR A	132	22.535	9.779	28.077	1.00 38.05
	MOTA	1080		THR A		20.792	7.731	26.746	1.00 38.81
	ATOM	1081		THR A		20.603	6.712	25.757	1.00 36.51
60	ATOM	1082		THR A		19.452	8.267	27.216	1.00 36.18
50	ATOM ATOM	1083 1084		ASN A ASN A		21.212 21.188	11.104 12.167	26.792 27.803	1.00 35.61 1.00 36.33
	ATOM	1085		ASN A		19.749	12.266	28.321	1.00 35.53
	MOTA	1086		ASN A		18.880	11.616	27.771	1.00 35.34

	7 004	1007	C.F.	א מיי	n 100		01			
	ATOM ATOM	1087			A 133		21.662			
	ATOM	1088			A 133		22.055		28.327	
	ATOM	1090		ASN .			22.192		27.956	
5	ATOM	1090			A 134		22.275		29.562	
	ATOM	1092			A 134		19.546 18.238		29.444 30.127	.1.00 35.65
	ATOM	1093			A 134		17.856		30.127	1.00 36.02 1.00 36.37
	ATOM	1094	ő		A 134		18.686		31.095	1.00 36.37
	ATOM	1095	СВ		A 134		18.363		31.423	1.00 37.57
10	ATOM	1096	CG		A 134		18.900		31.221	1.00 34.96
	ATOM	1097	CD1		A 134		20.214		31.363	1.00 35.18
	ATOM	1098	CD2				18.190	9.511	30.845	1.00 37.83
	ATOM	1099	NEl	TRP			20.350		31.103	1.00 33.83
	ATOM	1100	CE2	TRP A	A 134	•	19.121		30.802	1.00 34.86
15	MOTA	1101	CE3	TRP A	A 134		16.836		30.593	1.00 35.07
	MOTA	1102	CZ2	TRP A			18.770	7.136	30.516	1.00 36.92
	ATOM	1103	CZ3				16.498	7.932	30.308	1.00 39.28
	ATOM	1104		TRP A			17.449	6.905	30.240	1.00 38.59
20	ATOM	1105	N		A 135		16.634	14.807	30.259	1.00 36.82
20	ATOM	1106	CA	THR A			16.349	16.149	30.758	1.00 36.51
	ATOM	1107	C		1 135		16.094	16.125	32.270	1.00 37.13
	ATOM	1108	0	THR A			16.234	17.149	32.927	1.00 35.77
	ATOM	1109	CB		135	•	15.214	16.871	30.031	1.00 41.31
25	ATOM	1110		THR A			13.979	16.175	30.224	1.00 39.42
23	ATOM	1111		THR A			15.461	16.910	28.512	1.00 43.30
	ATOM	1112 1113	N	HIS F			15.650	15.007	32.831	1.00 36.50
	ATOM ATOM		CA	HIS F			15.236	14.974	34.227	1.00 37.55
	ATOM	1114 1115	C O	HIS F			16.017 15.783	13.856	34.948	1.00 36.41
30	ATOM	1116	СВ	HIS A			13.731	12.717 14.716	34.570	1.00 37.39
50	ATOM	1117	CG	HIS A			12.843	15.884	34.346	1.00 42.28 1.00 45.85
	ATOM	1118		HIS A			12.928	16.585	34.044 32.850	1.00 45.85
	ATOM	1119		HIS A			11.847	16.467	34.751	1.00 47.41
	ATOM	1120		HIS A			12.039	17.564	32.853	1.00 47.41
35	ATOM	1121		HIS A			11.362	17.512	33.987	1.00 49.47
	ATOM	1122	N	ILE A			16.941	14.223	35.827	1.00 35.44
	ATOM	1123	CA	ILE A			17.696	13.165	36.526	1.00 34.42
	ATOM	1124	С	ILE A			17.396	13.291	38.023	1.00 34.06
	MOTA	1125	0	ILE A	137 -		17.573	14.396	38.537	1.00 34.29
40	ATOM	1126	CB	ILE A	137		19.209	13.314	36.268	1.00 33.02
	ATOM	1127	CG1	ILE A	137		19.527	13.053	34.780	1.00 33.98
	ATOM	1128	CG2	ILE A			19.995	12.315	37.126	1.00 34.85
	ATOM	1129	CD1	ILE A			20.948	13.484	34.427	1.00 35.15
45	ATOM	1130	N	TYR A			16.902	12.217	38.643	1.00 33.90
43	MOTA	1131	CA	TYR A			16.497	12.371	40.067	1.00 34.35
	ATOM	1132	C	TYR A			17.618	11.920	40.998	1.00 34.35
	ATOM ATOM	1133 1134	O	TYR A			17.925	10.740	40.954	1.00 35.52
	ATOM	1135	CB	TYR A			15.196	11.604	40.319	1.00 35.05
50	ATOM	1136	CG CD1	TYR A				12.281	39.524	
50	ATOM	1137		TYR A			13.904 13.272	11.924	38.203	1.00 38.75 1.00 40.04
	ATOM	1138		TYR A			12.922	13.267 12.525	40.084	
	ATOM	1139		TYR A			12.281	13.870	37.431 39.308	1.00 39.64
	ATOM	1140		TYR A			12.128	13.492	37.999	1.00 41.81 1.00 41.16
55	ATOM	1141		TYR A			11.171	14.050	37.192	1.00 41.10
=	ATOM	1142	N	ILE A			18.255	12.823	41.721	1.00 43.38
	ATOM	1143		ILE A			19.360	12.458	42.607	1.00 34.48
	ATOM	1144		ILE A			18.756	12.127	43.996	1.00 34.60
4	ATOM	1145		ILE A			18.312	13.089	44.613	1.00 35.20
60	ATOM	1146		ILE A			20.353	13.612	42.774	1.00 34.61
	ATOM	1147		ILE A			20.926	14.098	41.421	1.00 38.01
	MOTA	1148		ILE A		ļi.	21.546	13.200	43.637	1.00 37.55
	ATOM	1149	CD1	ILE A	139		21.487	12.956	40.588	1.00 38.91

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	ATOM	1150				1 140	18.58		10.861	44.301		35.26
	ATOM	1151				140	17.93		10.511	45.590		37.11
	ATOM	1152				140	18.95		10.174	46.664		37.66
5	MOTA	1153 1154				140	19.86		9.384	46.448		37.82
J	MOTA MOTA	1154				140	17.07		9.251	45.411		42.45
	MOTA	1156	_			140	15.48		9.689	44.680		49.17
	ATOM	1157				141	18.79 19.66		10.796	47.831		37.14
	ATOM	1158				141	18.84		10.484	48.966		37.88
10	ATOM	1159				141	17.67		9.929 9.579	50.125		36.63
	ATOM	1160				141	20.50		11.709	49.925 49.297		35.72
	ATOM	1161				141	21.39		12.145	48.129		53.61
	ATOM	1162				141	22.12		13.446	48.352		58.09
	MOTA	1163		1 GLU			21.54		14.528	48.139		57.53
15	MOTA	1164		2 GLU			23.30		13.339	48.747		64.14
	ATOM	1165				142	19.44		9.883	51.315		36.78
	ATOM	1166	CA	GLU	Α	142	18.78		9.263	52.479		36.84
	MOTA	1167	С	GLU	Α	142	17.51	5	9.941	52.907		35.85
	ATOM	1168	0	GLU	Α	142	16.49	6	9.267	53.166		36.59
20	ATOM	1169	CB	GLU	Α	142	19.78	0	9.360	53.654	1.00	43.10
	ATOM	1170				142	21.15		8.763	53.466	1.00	54.03
	MOTA	1171	CD			142	22.32		9.696	53.311	1.00	60.55
	ATOM	1172	OE!	GLU	Α	142	22.26		10.679	52.543	1.00	59.21
25	ATOM	1173		GLU			23.40		9.470	53.924		64.17
25	ATOM	1174	N			143	17.47		11.272	52.922		34.96
	ATOM	1175	CA			143	16.24		11.960	53.308		36.52
	MOTA	1176	C			143	15.73		12.999	52.312		36.98
	MOTA MOTA	1177 1178	0			143	15.23		14.019	52.787		38.22
30	ATOM	1178	CB			143 144	16.56		12.620	54.652		34.45
50	MOTA	1180	N CA			144	16.16 15.75		12.881	51.031		36.01
	ATOM	1181	C			144	15.95		13.884 13.477	50.048 48.583		35.70
	ATOM	1182	ŏ			144	16.66		12.520	48.259		35.68 34.04
	ATOM	1183	ČВ			144	16.60		15.158	50.246		39.92
35	ATOM	1184	OG			144	17.96		14.791	49.965		46.64
	ATOM	1185	N			145	15.36		14.287	47.712		36.14
	ATOM	1186	CA	VAL			15.57		14.054	46.260		35.49
	ATOM	1187	С	VAL			15.54		15.410	45.563		36.78
	ATOM	1188	0	VAL			14.80		16.307	45.979		34.89
40	ATOM	1189	CB	VAL	Α	145	14.580	0	13.058	45.707		36.75
	MOTA	1190	CG1				13.143	1	13.446	46.028	1.00	36.76
	MOTA	1191	CG2				14.730	0	12.908	44.192		37.20
	MOTA	1192	N	THR			16.453		15.595	44.600	1.00	37.23
45	ATOM	1193	CA	THR			16.434		16.814	43.769		39.11
45	MOTA	1194	С	THR			16.529		16.390	42.297	1.00	39.36
	MOTA	1195	0	THR			17.361		15.521	41.981		39.50
	ATOM ATOM	1196	CB	THR			17.709		17.657	44.040		43.57
	ATOM	1197 1198	OG1				17.833		17.886	45.432		49.29
50	ATOM	1199		THR VAL						43.244		46.55
20	ATOM	1200	N CA	VAL			15.699 15.774		16.998	41.454		39.48
	ATOM	1201	C	VAL			16.800		16.719	40.017		38.72
	ATOM	1202	Õ	VAL			16.921		17.682	39.433		39.04
	ATOM	1203	СВ	VAL			14.451		18.842 16.800	39.851 39.268		38.28
55	ATOM	1204		VAL			13.871		18.209	39.197		40.51 42.34
	ATOM	1205		VAL			14.532		16.183	37.873		36.37
	ATOM	1206	N	VAL			17.711		17.103	38.634		39.16
	ATOM	1207	CA	VAL			18.685		17.909	37.910	1.00	38.86
	ATOM	1208	C	VAL			18.569		17.615	36.406		38.03
60	ATOM	1209	õ	VAL .			18.093		16.554	35.994		38.38
	ATOM	1210	CB	VAL :	A :	148	20.117		17.663	38.437		37.94
	ATOM	1211	CG1	VAL .	A :	148	20.196		17.921	39.948		37.81
	ATOM	1212	CG2	VAL A	A :	148	20.543		16.227	38.135		39.08

ATOM 1214 CA GLU A 149 19.010 18.272 34.118 1.00 37.6 ATOM 1216 O GLU A 149 20.309 17.767 33.517 1.00 36.4 ATOM 1216 O GLU A 149 18.519 19.530 33.403 1.00 48.9 ATOM 1217 CB GLU A 149 18.519 19.530 33.403 1.00 48.9 ATOM 1218 CG GLU A 149 19.598 20.527 33.046 1.00 53.6 ATOM 1219 CD GLU A 149 19.598 20.527 33.046 1.00 53.6 ATOM 1210 OE2 GLU A 149 19.100 21.544 32.022 1.00 58.0 ATOM 1221 OE2 GLU A 149 19.100 21.544 32.022 1.00 58.0 ATOM 1221 OE2 GLU A 149 18.363 21.228 31.067 1.00 55.3 ATOM 1222 OE1 GLU A 149 18.363 21.228 31.067 1.00 55.3 ATOM 1222 OE1 GLU A 149 18.363 21.228 31.067 1.00 55.3 ATOM 1223 CA GLY A 150 20.200 16.861 32.559 1.00 37.2 ATOM 1225 O GLY A 150 21.399 16.289 31.923 1.00 37.2 ATOM 1226 N GLN A 151 23.191 17.714 31.014 1.00 37.2 ATOM 1226 N GLN A 151 23.181 17.714 31.014 1.00 37.2 ATOM 1228 C GLN A 151 23.181 17.714 31.014 1.00 37.2 ATOM 1228 C GLN A 151 23.181 17.714 31.014 1.00 37.2 ATOM 1228 C GLN A 151 23.181 17.714 31.00 31.00 37.4 ATOM 1231 CG GLN A 151 24.280 19.937 31.078 1.00 37.4 ATOM 1231 CG GLN A 151 24.280 19.937 31.078 1.00 37.4 ATOM 1231 CG GLN A 151 23.181 17.70 32.581 1.00 37.4 ATOM 1233 OE1 GLN A 151 23.820 21.769 33.905 1.00 49.5 ATOM 1234 NE2 GLN A 151 23.820 21.769 33.905 1.00 49.5 ATOM 1234 NE2 GLN A 151 23.820 21.769 33.905 1.00 49.5 ATOM 1234 NE2 GLN A 151 23.820 21.769 33.905 1.00 49.5 ATOM 1236 CA VAL A 152 25.913 19.028 28.294 1.00 36.0 ATOM 1236 CA VAL A 152 26.997 18.488 27.284 1.00 36.0 ATOM 1237 C VAL A 152 25.9585 18.266 25.921 1.00 36.7 ATOM 1239 CB VAL A 152 25.9585 18.266 25.921 1.00 36.7 ATOM 1240 CG1 VAL A 152 25.985 18.266 25.921 1.00 36.7 ATOM 1240 CG1 VAL A 152 25.985 19.932 27.005 1.00 37.0 ATOM 1240 CG1 VAL A 152 25.985 19.932 27.005 1.00 37.0 ATOM 1240 CG2 VAL A 152 25.985 19.932 27.005 1.00 37.0 ATOM 1240 CG1 VAL A 152 25.985 19.932 27.005 1.00 36.7 ATOM 1247 CG ASP A 153 30.980 20.514 28.634 1.00 36.7 ATOM 1247 CG ASP A 153 30.980 20.514 28.634 1.00 36.7 ATOM 1245 CD ASP A 153 30.980 20.514 28.634 1.00 36.7 ATOM 1245 CD ASP A 153 30.980 20.514 28.63	4575406938521267668625012754117
ATOM	596006938521267668625012754117
S	96034425629425475108271060917
ATOM	600344256294276686250127754117
ATOM	034442562942547551082711060917
ATOM 1220 OE1 GLU A 149 19.440 22.716 32.229 1.00 55.3 ATOM 1221 OE2 GLU A 149 18.363 21.228 31.067 1.00 61.4 ATOM 1222 N GLY A 150 20.200 16.861 32.559 1.00 37.4 ATOM 1223 CA GLY A 150 21.399 16.289 31.923 1.00 37.5 ATOM 1225 O GLY A 150 21.910 17.392 30.970 1.00 37.5 ATOM 1226 N GLN A 151 23.181 17.714 31.014 1.00 37.5 ATOM 1227 CA GLN A 151 23.713 18.812 30.210 1.00 36.0 ATOM 1228 C GLN A 151 23.713 18.812 30.210 1.00 36.0 ATOM 1229 O GLN A 151 24.833 18.247 29.331 1.00 37.4 ATOM 1229 O GLN A 151 25.351 17.166 29.610 1.00 35.2 ATOM 1230 CB GLN A 151 23.177 20.667 31.852 1.00 43.4 ATOM 1231 CG GLN A 151 23.177 20.667 31.852 1.00 43.4 ATOM 1233 OE1 GLN A 151 23.987 22.896 31.946 1.00 49.7 ATOM 1233 OE1 GLN A 151 23.987 22.896 31.946 1.00 49.7 ATOM 1234 NE2 GLN A 151 23.987 22.896 31.946 1.00 49.7 ATOM 1235 C VAL A 152 25.173 19.028 28.294 1.00 36.0 ATOM 1237 C VAL A 152 25.097 18.488 27.284 1.00 36.0 ATOM 1237 C VAL A 152 25.097 18.488 27.284 1.00 36.0 ATOM 1239 CB VAL A 152 25.385 18.266 25.921 1.00 40.1 ATOM 1239 CB VAL A 152 25.385 18.266 25.921 1.00 40.1 ATOM 1240 CGI VAL A 152 25.385 18.266 25.921 1.00 37.0 ATOM 1240 CGI VAL A 152 25.385 18.266 25.921 1.00 37.0 ATOM 1240 CGI VAL A 152 25.385 18.266 25.921 1.00 37.0 ATOM 1240 CG VAL A 152 25.385 18.266 25.921 1.00 37.0 ATOM 1240 CG VAL A 152 25.385 18.266 25.921 1.00 37.0 ATOM 1240 CG VAL A 152 25.385 18.266 25.921 1.00 37.0 ATOM 1240 CG VAL A 152 25.385 18.266 25.921 1.00 37.0 ATOM 1240 CG VAL A 152 26.994 17.345 25.148 1.00 37.0 ATOM 1240 CG VAL A 152 26.994 17.345 25.148 1.00 37.0 ATOM 1240 CG VAL A 152 26.994 17.345 25.148 1.00 37.0 ATOM 1240 CG VAL A 152 26.994 17.345 25.148 1.00 37.0 ATOM 1240 CG VAL A 152 26.994 17.345 25.148 1.00 37.0 ATOM 1240 CG VAL A 153 30.452 19.060 25.554 1.00 36.7 ATOM 1240 CG VAL A 153 30.452 19.060 25.554 1.00 36.7 ATOM 1245 O ASP A 153 30.452 19.060 25.554 1.00 37.0 ATOM 1245 O ASP A 153 30.452 19.060 25.554 1.00 36.7 ATOM 1245 O ASP A 153 30.452 19.060 25.554 1.00 38.8 ATOM 1245 O ASP	3493852126766862771754117
10 ATOM 1221 OE2 GLU A 149 18.363 21.226 31.067 1.00 61.4 ATOM 1222 N GLY A 150 20.200 16.861 32.559 1.00 37.4 ATOM 1223 CA GLY A 150 21.399 16.289 31.923 1.00 37.5 ATOM 1224 C GLY A 150 21.910 17.392 30.970 1.00 37.5 ATOM 1225 O GLY A 150 21.910 17.392 30.970 1.00 37.5 ATOM 1226 N GLN A 151 23.181 17.714 31.014 1.00 37.2 ATOM 1227 CA GLN A 151 23.181 17.714 31.014 1.00 37.2 ATOM 1228 C GLN A 151 23.713 18.812 30.210 1.00 36.9 ATOM 1229 O GLN A 151 24.833 18.247 29.331 1.00 37.5 ATOM 1229 O GLN A 151 24.833 18.247 29.331 1.00 37.5 ATOM 1230 CB GLN A 151 22.3551 17.166 29.610 1.00 35.2 ATOM 1231 CG GLN A 151 23.181 17.714 31.014 1.00 37.5 ATOM 1231 CG GLN A 151 23.177 20.667 31.852 1.00 43.4 ATOM 1232 CD GLN A 151 23.987 22.896 31.946 1.00 48.7 ATOM 1233 OE1 GLN A 151 23.987 22.896 31.946 1.00 48.7 ATOM 1233 OE1 GLN A 151 23.987 22.896 31.946 1.00 48.7 ATOM 1235 N VAL A 152 23.987 22.896 31.946 1.00 49.5 ATOM 1235 N VAL A 152 25.173 19.028 28.294 1.00 36.0 ATOM 1236 CA VAL A 152 26.949 20.667 26.795 1.00 36.7 ATOM 1238 O VAL A 152 27.209 19.494 26.986 1.00 37.2 ATOM 1239 CB VAL A 152 26.949 20.667 26.795 1.00 36.7 ATOM 1239 CB VAL A 152 26.949 20.667 26.795 1.00 36.7 ATOM 1240 CG1 VAL A 152 26.949 20.667 26.795 1.00 36.7 ATOM 1240 CG1 VAL A 152 26.949 20.667 26.795 1.00 36.7 ATOM 1240 CG1 VAL A 152 26.949 20.667 26.795 1.00 36.7 ATOM 1240 CG1 VAL A 152 26.949 20.667 26.795 1.00 37.0 ATOM 1241 CG2 VAL A 152 26.394 17.345 25.148 1.00 37.0 ATOM 1242 N ASP A 153 30.496 17.345 25.148 1.00 37.0 ATOM 1244 C ASP A 153 30.496 17.903 27.005 1.00 37.6 ATOM 1247 CG ASP A 153 30.890 20.514 28.634 1.00 37.0 ATOM 1248 OD1 ASP A 153 30.990 20.514 28.634 1.00 37.6 ATOM 1248 OD1 ASP A 153 30.990 20.514 28.634 1.00 37.6 ATOM 1245 O ASP A 153 30.990 20.514 28.634 1.00 37.6 ATOM 1247 CG ASP A 153 30.990 20.514 28.634 1.00 37.0 ATOM 1248 OD1 ASP A 153 30.990 20.514 28.634 1.00 37.0 ATOM 1245 O ASP A 153 30.990 20.514 28.634 1.00 37.0 ATOM 1246 CB ASP A 153 30.990 20.514 28.634 1.00 37.0 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.	4938521267668625012754117
10 ATOM 1222 N GLY A 150 20.200 16.861 32.559 1.00 37.4 ATOM 1224 C GLY A 150 21.399 16.289 31.923 1.00 37.4 ATOM 1224 C GLY A 150 21.910 17.392 30.970 1.00 37.5 ATOM 1225 O GLY A 150 21.910 17.392 30.970 1.00 37.6 ATOM 1226 N GLN A 151 23.181 17.714 31.014 1.00 37.6 ATOM 1227 CA GLN A 151 23.181 17.714 31.014 1.00 37.6 ATOM 1228 C GLN A 151 23.713 18.812 30.210 1.00 36.9 ATOM 1229 O GLN A 151 24.833 18.247 29.331 1.00 37.4 ATOM 1220 C GLN A 151 25.351 17.166 29.610 1.00 35.2 ATOM 1230 CB GLN A 151 25.351 17.166 29.610 1.00 37.5 ATOM 1231 CG GLN A 151 23.177 20.667 31.852 1.00 43.4 ATOM 1232 CD GLN A 151 23.177 20.667 31.852 1.00 43.4 ATOM 1233 OE1 GLN A 151 23.987 22.896 31.946 1.00 49.5 ATOM 1234 NE2 GLN A 151 23.820 21.769 33.905 1.00 44.1 ATOM 1235 N VAL A 152 25.173 19.028 28.294 1.00 36.0 ATOM 1237 C VAL A 152 25.173 19.028 28.294 1.00 36.0 ATOM 1237 C VAL A 152 25.173 19.028 28.294 1.00 36.0 ATOM 1238 O VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1239 CB VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1239 CB VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1230 CB VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1237 C VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1238 O VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1238 O VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1237 C VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1241 CG2 VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.488 27.284 1.00 36.7 ATOM 1240 CGI VAL A 152 26.097 18.489 20.0667 26.095 1.00 36.0 ATOM 1240 CGI VAL A 152 26.097 18.488 2	438552126766862508277154117
ATOM 1223 CA GLY A 150 21.399 16.289 31.923 1.00 37.2 ATOM 1224 C GLY A 150 21.910 17.392 30.970 1.00 37.5 ATOM 1225 O GLY A 150 21.071 18.016 30.338 1.00 37.6 ATOM 1226 N GLN A 151 23.181 17.714 31.014 1.00 37.5 ATOM 1227 CA GLN A 151 23.713 18.812 30.210 1.00 36.7 ATOM 1228 C GLN A 151 224.833 18.247 29.331 1.00 37.4 ATOM 1229 O GLN A 151 25.351 17.166 29.610 1.00 35.2 ATOM 1230 CB GLN A 151 25.351 17.166 29.610 1.00 35.2 ATOM 1231 CG GLN A 151 23.177 20.667 31.852 1.00 37.5 ATOM 1232 CD GLN A 151 23.987 32.581 1.00 48.7 ATOM 1233 OE1 GLN A 151 23.987 32.581 1.00 48.7 ATOM 1234 NE2 GLN A 151 23.987 32.896 31.946 1.00 49.5 ATOM 1235 N VAL A 152 23.987 22.896 31.946 1.00 48.7 ATOM 1236 CA VAL A 152 25.173 19.028 28.294 1.00 36.8 ATOM 1237 C VAL A 152 26.097 18.488 27.284 1.00 36.8 ATOM 1238 O VAL A 152 26.949 20.667 67 66.795 1.00 40.1 ATOM 1239 CB VAL A 152 26.949 20.667 67 66.795 1.00 37.2 ATOM 1239 CB VAL A 152 26.949 20.667 67 60.88 1.00 37.0 ATOM 1240 CG1 VAL A 152 26.394 17.345 25.148 1.00 37.0 ATOM 1240 CG1 VAL A 152 26.394 17.345 25.148 1.00 37.0 ATOM 1241 CG2 VAL A 152 26.394 17.345 25.148 1.00 37.0 ATOM 1244 CA ASP A 153 30.452 19.060 25.554 1.00 37.9 ATOM 1245 CA ASP A 153 30.452 19.060 25.554 1.00 37.9 ATOM 1246 CB ASP A 153 30.492 19.23 27.005 1.00 37.9 ATOM 1247 CG ASP A 153 30.492 19.23 28.066 1.00 37.9 ATOM 1248 OD1 ASP A 153 30.492 19.23 28.066 1.00 37.9 ATOM 1249 OD2 ASP A 153 30.890 20.514 28.634 1.00 39.4 ATOM 1249 OD2 ASP A 153 30.499 21.441 27.840 1.00 37.6 ATOM 1249 OD2 ASP A 153 30.499 21.441 27.840 1.00 36.7 ATOM 1250 N TYR A 154 31.550 19.785 25.263 1.00 36.7 ATOM 1250 C TYR A 154 33.386 16.934 24.276 1.00 38.7 ATOM 1255 C TYR A 154 33.386 16.934 24.276 1.00 38.7 ATOM 1255 C TYR A 154 33.624 20.200 23.920 1.00 38.7 ATOM 1255 CD TYR A 154 33.624 20.200 23.920 1.00 38.7 ATOM 1255 CD TYR A 154 33.624 20.200 23.920 1.00 38.7	255621267668622771754117
ATOM 1225 C GLY A 150 21.910 17.392 30.970 1.00 37.5 ATOM 1225 O GLY A 150 21.071 18.016 30.338 1.00 37.5 ATOM 1226 N GLN A 151 23.181 17.714 31.014 1.00 37.2 15 ATOM 1227 CA GLN A 151 23.713 18.812 30.210 1.00 36.9 ATOM 1228 C GLN A 151 24.833 18.247 29.331 1.00 37.4 ATOM 1229 O GLN A 151 24.833 18.247 29.331 1.00 37.5 ATOM 1230 CB GLN A 151 24.280 19.937 31.078 1.00 37.5 ATOM 1231 CG GLN A 151 23.177 20.667 31.852 1.00 43.4 ATOM 1232 CD GLN A 151 23.177 20.667 31.852 1.00 43.4 ATOM 1233 OE1 GLN A 151 23.691 21.877 32.581 1.00 48.7 ATOM 1233 OE1 GLN A 151 23.820 21.769 33.905 1.00 44.1 ATOM 1235 N VAL A 152 25.173 19.028 28.294 1.00 36.8 ATOM 1235 C VAL A 152 25.173 19.028 28.294 1.00 36.8 ATOM 1238 O VAL A 152 26.097 18.488 27.284 1.00 36.8 ATOM 1239 CB VAL A 152 26.097 18.468 27.284 1.00 36.8 ATOM 1239 CB VAL A 152 26.394 17.345 25.148 1.00 37.0 ATOM 1240 CG1 VAL A 152 26.394 17.345 25.148 1.00 37.0 ATOM 1241 CG2 VAL A 152 26.394 17.345 25.148 1.00 37.0 ATOM 1242 C ASP A 153 30.452 19.060 25.554 1.00 37.0 ATOM 1244 C ASP A 153 30.452 19.060 25.554 1.00 37.9 ATOM 1245 C ASP A 153 30.452 19.060 25.554 1.00 37.9 ATOM 1246 CB ASP A 153 30.452 19.060 25.554 1.00 37.9 ATOM 1247 CG ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1247 CG ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.00 36.7 ATOM 1248 OD1 ASP A 153 30.469 21.441 20.767 29.695 1.00 38.7 ATOM 1250 C TYR A 154 33.624 20.200 23.920 1.00 38.9 ATOM 1250 C TYR A 154 33.624 20.200 23.920 1.00 38.9 ATOM 1250 C TYR A 154 33.624 20.200 23.920 1.00 38.9 ATOM 1255 CG TYR A 154 34.637 19.489 23.038 1.00 38.9	5521296766862127754117 60117
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30 ATOM 1242 N ASP A 153 28.420 19.032 27.005 1.00 37.0 ATOM 1243 CA ASP A 153 29.712 19.530 26.819 1.00 37.9 ATOM 1244 C ASP A 153 30.452 19.060 25.554 1.00 36.1 ATOM 1245 O ASP A 153 30.094 18.059 24.955 1.00 37.6 ATOM 1246 CB ASP A 153 30.713 19.123 28.066 1.00 30.7 ATOM 1247 CG ASP A 153 30.890 20.514 28.634 1.00 39.4 ATOM 1248 OD1 ASP A 153 30.469 21.441 27.840 1.00 53.6 ATOM 1249 OD2 ASP A 153 31.411 20.767 29.695 1.00 41.0 ATOM 1250 N TYR A 154 31.550 19.785 25.263 1.00 36.7 ATOM 1251 CA TYR A 154 32.497 19.232 24.299 1.00 38.0 ATOM 1252 C TYR A 154 33.386 16.934 24.276 1.00 38.7 ATOM 1253 O TYR A 154 33.386 16.934 24.276 1.00 38.7 ATOM 1255 CG TYR A 154 33.624 20.200 23.920 1.00 38.3 ATOM 1255 CG TYR A 154 34.637 19.489 23.038 1.00 38.7 ATOM 1255 CG TYR A 154 34.637 19.489 23.038 1.00 38.7 ATOM 1255 CG TYR A 154 34.295 19.193 21.714 1.00 39.8	01 91 17
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45 XMOM 1957 CD2 MVD X 154 - 25 075 10 104 22 514 1 00 20 5	
ATOM 1258 CE1 TYR A 154 35.184 18.532 20.873 1.00 39.9	
ATOM 1259 CE2 TYR A 154 36.759 18.454 22.687 1.00 41.2	
ATOM 1260 CZ TYR A 154 36.412 18.174 21.376 1.00 41.1	
ATOM 1261 OH TYR A 154 37.332 17.516 20.610 1.00 42.1	
50 ATOM 1262 N TYR A 155 33.319 18.027 26.224 1.00 38.1	١3
ATOM 1263 CA TYR A 155 33.883 16.968 27.018 1.00 38.8	
ATOM 1264 C TYR A 155 32.959 15.819 27.350 1.00 37.80	
ATOM 1265 O TYR A 155 33.530 14.735 27.543 1.00 37.7	
ATOM 1266 CB TYR A 155 34.500 17.518 28.323 1.00 40.00)3
55 ATOM 1267 CG TYR A 155 35.364 18.745 28.031 1.00 43.79	15
ATOM 1268 CD1 TYR A 155 34.854 20.021 28.230 1.00 44.6	54
ATOM 1269 CD2 TYR A 155 36.655 18.604 27.562 1.00 44.80	16
ATOM 1270 CE1 TYR A 155 35.628 21.136 27.950 1.00 46.5	5
ATOM 1271 CE2 TYR A 155 37.440 19.709 27.271 1.00 46.3	
60 ATOM 1272 CZ TYR A 155 36.920 20.963 27.485 1.00 48.0)4
ATOM 1273 OH TYR A 155 37.708 22.064 27.230 1.00 50.62	
ATOM 1274 N GLY A 156 31.651 16.005 27.491 1.00 36.89	
ATOM, 1275 CA GLY A 156 30.784 14.894 27.833 1.00 36.2	

	ATOM	1276	С	GLY A	156		29.374	15.297	28.278	1.00 36.29
	ATOM	1277	0	GLY A	156		28.845	16.351	27.962	1.00 36.73
	ATOM	1278	N	LEU A	157		28.737	14.367	28.989	1.00 35.47
	ATOM	1279	CA	LEU A	157		27.410	14.593	29.547	1.00 36.71
5	ATOM	1280	С	LEU A	157		27.570	14.782	31.061	1.00 36.98
	MOTA	1281	0	LEU A	157		28.299	14.009	31.703	1.00 37.91
	ATOM	1282	CB	LEU A	. 157		26.472	13.404	29.348	1.00 36.06
	MOTA	1283	CG	LEU A	157		26,409	12.902	27.878	1.00 39.11
	ATOM	1284	CD1	LEU A	157		25.362	11.777	27.835	1.00 40.34
10	MOTA	1285	CD2	LEU A	157		25.944	14.021	26.948	1.00 37.66
	ATOM	1286	N	TYR A	158		26.860	15.773	31.583	1.00 36.59
	ATOM	1287	CA	TYR A	158		27.043	16.018	33.020	1.00 37.29
	MOTA	1288	С	TYR A	158		25.778	16.579	33.654	1.00 37.06
	MOTA	1289	0	TYR A	158		24.813	16.941	32.968	1.00 36.78
15	MOTA	1290	CB	TYR A	158		28.202	17.007	33.172	1.00 37.24
	MOTA	1291	CG	TYR A			27.948	18.410	32.664	1.00 38.25
	ATOM	1292	CD1			-	27.547	19.427	33.526	1.00 37.59
	ATOM	1293		TYR A			28.158	18.721	31.322	1.00 38.51
	ATOM	1294	CE1				27.355	20.718	33.056	1.00 38.42
20	ATOM	1295	CE2				27.955	20.009	30.839	1.00 38.37
	ATOM	1296	CZ	TYR A			27.573	21.006	31.711	1.00 38.61
	ATOM	1297	OH	TYR A			27.359	22.290	31.260	1.00 37.90
	ATOM	1298	N	TYR A			25.799	16.661	34.979	1.00 36.65
	ATOM	1299	CA	TYR A			24.758	17.394	35.694	1.00 37.45
25	ATOM	1300	C	TYR A	-		25.493	18.169	36.801	1.00 37.16
45	ATOM	1301	Ö	TYR A			26.659	17.920	37.045	1.00 37.16
	ATOM	1302	СВ	TYR A			23.638	16.543	36.301	1.00 37.10
	ATOM	1303	CG	TYR A			24.161	15.441	37.222	1.00 37.42
	ATOM	1303	CD1				24.429	14.181	36.732	1.00 37.33
30	ATOM	1304	CD2	TYR A			24.352	15.689	38.574	1.00 39.31
50	ATOM	1305	CE1	TYR A			24.902	13.169	37.564	1.00 39.89
	ATOM	1307	CE2	TYR A			24.823	14.699	39.407	1.00 39.69
		1307	CZ	TYR A			25.101	13.454	38.893	1.00 38.54
	ATOM	1309	OH	TYR A			25.613		39.741	1.00 40.63
35	ATOM							12.488	37.356	1.00 36.88
55	ATOM	1310 1311	N CA	VAL A			24.779	19.122	38.452	1.00 38.80
	MOTA	1311	CA	VAL A			25.251 24.277	19.943 19.714		1.00 38.20
	ATOM			VAL A					39.629	
	ATOM	1313	0	VAL A			23.078	19.922	39.514	1.00 38.89
40	MOTA	1314	CB	VAL A			25.295	21.439	38.094	1.00 41.01
40	ATOM	1315		VAL A			25.815 26.254	22.251	39.288	1.00 39.83
	ATOM	1316		VAL A				21.687	36.916	1.00 36.61
	ATOM	1317	И	HIS A			24.818	19.208	40.708	1.00 39.08
	ATOM	1318	CA	HIS A			24.018	18.916	41.919	1.00 39.84
45	ATOM	1319	C	HIS A			24.734	19.569	43.095	1.00 39.51
43	MOTA	1320	0		161		25.900	19.316	43.322	1.00 38.92
	MOTA	1321	CB	HIS A			23.939	17.418	42.140	1.00 37.10
	ATOM	1322	CG		161		23.189	16.976	43.377	1.00 36.87
	ATOM	1323	ND1	HIS A			21.908	17.363	43.665	1.00 42.27
50	ATOM	1324		HIS A			23.571	16.163	44.374	1.00 38.66
30	ATOM	1325		HIS A			21.508	16.811	44.805	1.00 34.42
	ATOM	1326		HIS A			22.503	16.079	45.262	1.00 40.76
	ATOM	1327	N	GLU A			24.031	20.404	43.832	1.00 41.45
	ATOM	1328	CA	GLU A			24.557	21.115	44.998	1.00 43.07
	ATOM	1329	С	GLU A			25.795	21.928	44.616	1.00 42.85
55	ATOM	1330	0	GLU A			26.806	21.828	45.304	1.00 43.43
	ATOM	1331	CB	GLU A			24.930	20.138	46.121	1.00 46.97
	MOTA	1332	CG	GLU A			23.750	19.235	46.415	1.00 59.55
	ATOM	1333	CD	GLU A			23.494	18.891	47.854	1.00 61.68
	ATOM	1334		GLU A			22.551	19.508	48.387	1.00 66.02
60	MOTA	1335	OE2	GLU A			24.226	18.027	48.364	1.00 65.49
	MOTA	1336	N	GLY A	163		25.786	22.518	43.432	1.00 43.79
	MOTA	1337	CA	GLY A	163		26.930	23.253	42.929	1.00 43.51
	MOTA	1338	С	GLY A	163		28.023	22.409	42.306	1.00 43.73
	7									

	MOTA	1339	0	GLY	A	163	28.958	23.011	41.746	1.00 43.41
	ATOM	1340	N	ILE	: A	164	27.986	21.079	42.371	1.00 42.17
	ATOM	1341	CA	ILE	: A	164	29.078	20.258	41.896	1.00 41.52
	MOTA	1342	C	ILE	: A	164	28.743	19.687	40.513	1.00 41.11
5	MOTA	1343	0	ILE	: A	164	27.677	19.110	40.314	1.00 40.21
	MOTA	1344	СВ	ILE	A	164	29.442	19.081	42.820	1.00 41.77
	ATOM	1345	CG1		: A	164	29.730	19.597	44.228	1.00 46.60
	ATOM	1346	CG2			164	30.651	18.346	42.258	1.00 43.25
	ATOM	1347	CD1			164	29.708	18.526	45.303	1.00 50.89
10	MOTA	1348	И			165	29.613	20.004	39.561	1.00 40.27
	ATOM	1349	CA			165	29.428	19.508	38.202	1.00 40.37
	ATOM	1350	C			165	29.979	18.082	38.132	1.00 40.18
	ATOM	1351	0			165	31.139	17.889	38.436	1.00 40.87
15	MOTA	1352	СВ			165	30.211	20.389	37.205	1.00 43.98
15	MOTA	1353	CG			165	30.190	19.775	35.799	1.00 48.81
	ATOM	1354	CD			165	31.056	20.614	34.844	1.00 50.67
	ATOM	1355	NE			165	30.374	21.882	34.644	1.00 54.50
	ATOM	1356	CZ			165	30.245	22.592	33.535	1.00 51.25
30	MOTA	1357		ARG			30.788	22.211	32.399	1.00 52.55
20	MOTA	1358		ARG			29.552	23.727	33.612	1.00 46.13
	ATOM	1359	N			166	29.159	17.127	37.747	1.00 38.84
	ATOM	1360	CA			166	29.502	15.722	37.710	1.00 37.91
	MOTA	1361	C			166	29.318	15.152	36.310	1.00 36.66
25	MOTA	1362	0			166	28.167	15.109	35.857	1.00 36.77
23	MOTA	1363	CB			166	28.621	14.911	38.700	1.00 42.71
	ATOM	1364		THR			28.895	15.399	40.034	1.00 43.09
	ATOM	1365		THR			28.934	13.427	38.662	1.00 40.93
	MOTA	1366	N			167	30.398	14.733	35.667	1.00 36.29
30	MOTA	1367	CA			167	30.309	14.112	34.342	1.00 36.95
50	ATOM	1368	С			167	29.970	12.639	34.466	1.00 37.76
	MOTA	1369	0			167	30.561	11.961	35.335	1.00 39.69
	ATOM	1370	CB			167	31.611	14.231	33.518	1.00 37.91
	ATOM ATOM	1371 1372	CG CD1			167	31.797 32.311	15.617	32.933	1.00 38.45
35	ATOM	1373		TYR TYR			32.311	16.637 15.937	33.726	1.00 39.32
55	ATOM	1374		TYR			32.458	17.919	31.646 33.243	1.00 39.69
	ATOM	1375	CE2				31.535	17.214	31.133	1.00 38.98 1.00 39.08
	ATOM	1376	CZ			167	32.064	18.201	31.133	1.00 40.35
	MOTA	1377	OH			167	32.216	19.488	31.494	1.00 40.33
40	ATOM	1378	N			168	28.924	12.172	33.821	1.00 33.01
	ATOM	1379	CA	PHE			28.547	10.772	33.818	1.00 37.39
	ATOM	1380	c.	PHE			28.987	10.058	32.559	1.00 39.29
	ATOM	1381	ŏ	PHE			28.980	8.825	32.494	1.00 38.30
	ATOM	1382	CB	PHE			27.085	10.508	34.167	1.00 38.07
45	ATOM	1383	CG	PHE			26.068	11.226	33.320	1.00 34.93
	ATOM	1384		PHE			25.596	10.661	32.153	1.00 36.11
	ATOM	1385		PHE			25.609	12.470	33.722	1.00 35.04
	ATOM	1386		PHE			24.656	11.337	31.364	1.00 34.93
	ATOM	1387		PHE			24.672	13.140	32.951	1.00 35.38
50	ATOM	1388	CZ				24.215			1.00 30.80
	ATOM	1389	N	VAL	Α	169	29.331	10.849	31.524	1.00 39.59
	MOTA	1390	CA	VAL			30.019	10.310	30.354	1.00 40.03
	ATOM	1391	С	VAL			31.149	11.322	30.039	1.00 41.32
	ATOM	1392	0	VAL	A	169		12.530	30.018	1.00 39.98
55	ATOM	1393	CB	VAL			29.136	10.155	29.112	1.00 39.59
	MOTA	1394		VAL	A	169	29.988	9.684	27.917	1.00 41.55
	ATOM	1395		VAL			28.019	9.107	29.242	1.00 38.14
•	ATOM	1396	N	GLN			32.377	10.844	29.870	1.00 41.92
	MOTA	1397	CA	GLN				11.693	29.396	1.00 42.70
60	ATOM	1398	C	GLN			33.833	11.215	27.990	1.00 43.33
	MOTA	1399	0	GLN	Α	170	34.348	10.097	27.861	1.00 43.22
	ATOM	1400	CB	GLN				11.627	30.293	1.00 39.48
	ATOM .	1401	CG	GLN	Ą	170		12.220	31.676	1.00 45.31

	MOTA	1402	CD	GLN A		35.691	12.212	32.542		46.68
	MOTA	1403		GLN A		35.649	11.848	33.717		52.69
	ATOM	1404	NE2			36.816	12.618	31.998		47.58
5	ATOM	1405	N	PHE A		33.678	12.076	26.982		43.04
)	ATOM	1406	CA	PHE A		33.884	11.606	25.629		44.34 45.84
	MOTA	1407 1408	C	PHE A		35.302	11.186	25.340		45.10
	MOTA MOTA	1400	O CB	PHE A		35.508 33.422	10.343 12.612	24.446 24.597		39.68
	MOTA	1410	CG	PHE A		31.961	12.978	24.537		38.24
10	ATOM	1411		PHE A		31.016	11.986	24.835		40.47
10	ATOM	1412		PHE A		31.530	14.269	24.673		35.50
	ATOM	1413		PHE A		29.673	12.310	24.912		37.70
	ATOM	1414		PHE A		30.187	14.604	24.441		37.70
	ATOM	1415	CZ	PHE A		29.248	13.621	24.690		37.99
15	MOTA	1416	N	LYS A		36.287	11.662	26.080		45.69
	ATOM	1417	CA	LYS A		37.660	11.223	25.889		47.54
	ATOM	1418	Ç	LYS A		37.949	9.748	26.138		48.27
	ATOM	1419	ŏ	LYS A		38.884	9.175	25.570		48.26
	ATOM	1420	CB	LYS A		38.594	12.102	26.708		52.42
20	ATOM	1421	CG	LYS A		40.022	12.159	26.201		57.12
	ATOM	1422	CD	LYS A		40.904	12.971	27.157		64.24
	ATOM	1423	CE	LYS A		42.362	12.543	27.018		65.59
	MOTA	1424	NZ	LYS A		43.304	13.691	26.949		65.87
	ATOM	1425	N	ASP A		37.154	9.132	27.009		48.25
25	ATOM	1426	CA	ASP A		37.212	7.712	27.287		49.23
	ATOM	1427	C	ASP A		36.954	6.925	26.007		49.36
	ATOM	1428	Ō	ASP A		37.788	6.072	25.701		49.13
	MOTA	1429	CB	ASP A		36.263	7.269	28.394		46.27
	MOTA	1430	, CG	ASP A	173	36.627	7.869	29.740	1.00	50.82
30	MOTA	1431	OD1			35.740	8.056	30.605	1.00	51.86
	MOTA	1432	OD2	ASP A	173	37.817	8.158	29.970	1.00	52.02
	MOTA	1433	N	ASP A	174	35.901	7.144	25.248	1.00	49.89
	ATOM	1434	CA	ASP A	174	35.671	6.430	24.007	1.00	50.79
	ATOM	1435	С	ASP A	174	36.647	6.784	22.897	1.00	52.00
35	MOTA	1436	0	ASP A	174	37.085	5.884	22.165	1.00	51.37
	MOTA	1437	CB	ASP A	174	34.231	6.582	23.539	1.00	51.65
,	MOTA	1438	CG	ASP A	174	33.276	5.662	24.274	1.00	51.83
	MOTA	1439	OD1	ASP A	174	33.751	4.664	24.847	1.00	48.40
	MOTA	1440	OD2	ASP A	174	32.060	5.942	24.269	1.00	52.72
40	ATOM	1441	N	ALA A	175	37.040	8.053	22.808	1.00	52.36
	ATOM	1442	CA	ALA A	175	38.024	8.476	21.821	1.00	53.78
	ATOM	1443	С	ALA A		39.362	7.759	21.964	1.00	54.22
	ATOM	1444	0	ALA A		39.999	7.417	20.974		54.32
4.5	ATOM	1445	CB	ALA A		38.226	9.986	21.910		51.67
45	MOTA	1446	N	GLU A 1		39.832	7.508	23.186		55.55
	MOTA	1447	CA		176	41.120	6.865	23.409		56.73
	MOTA	1448	С	GLU A 1		41.015	5.357	23.234		57.74
	ATOM	1449	0	GLU A 1		42.025	4.646	23.187		58.14
σ Ω (ATOM	1450	СВ	GLU A 1		41.655	7.170	24.806		56.85
50	ATOM	1451	CG	GLU A 1		41.910	8.632	25.116		59.30
	ATOM	1452	CD	GLU A 1		42.180	8.743	26.537		99.00
	MOTA	1453		GLU A 1		41.740	8.063	27.454		99.00
	MOTA	1454		GLU A 1		43.073	9.574	26.687		99.00
55	MOTA	1455	N	LYS A 1		39.790	4.852	23.170		58.44
55	ATOM	1456	CA	LYS A 1		39.555	3.420	23.024		59.70
	ATOM	1457	C	LYS A 1		39.312	3.069	21.561		60.20
	ATOM	1458	0	LYS A 1		39.326	1.895	21.198		60.71
	ATOM	1459	CB	LYS A 1		38.350	3.040	23.887		63.58
60	ATOM	1460	CG	LYS A 1		38.054	1.569	24.029		67.87
oo	ATOM	1461	CD	LYS A 1		37.047	1.277	25.140		70.02
	ATOM	1462	CE	LYS A 1		36.872	-0.235	25.242		73.46
	ATOM	1463	NZ	LYS A 1		36.221	-0.638	26.517		75.57
	ATOM	1464	N	TYR A 1	. 70	38.908	4.057	20.758	1.00	60.36

	ATOM MOTA	1465 1466	CA C	TYR A		38.551 39.369	3.798 4.563	19.381 18.361	1.00 61.69 1.00 62.23
	ATOM	1467	0	TYR A		39.821	3.923	17.409	1.00 63.37
	ATOM	1468	CB	TYR A		37.057	3.988	19.100	1.00 61.34
5	ATOM	1469	CG	TYR A	178	36.139	3.197	20.010	1.00 61.39
	ATOM	1470	CD1	TYR A	178	36.249	1.811	20.081	1.00 62.10
	MOTA	1471	CD2	TYR A	178	35.189	3.821	20.798	1.00 61.28
	MOTA	1472	CE1			35.440	1.072	20.929	1.00 62.32
10	MOTA	1473	CE2			34.378	3.097	21.651	1.00 62.22
10	ATOM	1474	CZ	TYR A		34.505		21.707	1.00 62.51
	ATOM	1475	OH	TYR F		33.696	0.989	22.540	1.00 62.15
	ATOM	1476	N	SER A		39.573	5.858	18.525	1.00 62.95
	ATOM ATOM	1477 1478	CA C.	SER F		40.159 41.662	6.703 6.923	17.498 17.631	1.00 64.19 1.00 64.98
15	ATOM	1479	0	SER A		42.279	6.550	18.630	1.00 64.79
1.5	ATOM	1480	СВ	SER A		39.470	8.077	17.505	1.00 65.34
	ATOM	1481	OG	SER A		39.982	8.923	16.491	1.00 69.64
	ATOM	1482	N	LYS A		42.254	7.552	16.609	1.00 65.75
	ATOM	1483	CA	LYS A		43.672	7.876	16.658	1.00 66.93
20	MOTA	1484	С	LYS A		43.886	9.316	17.107	1.00 67.25
	ATOM	1485	0	LYS A	180	44.806	9.591	17.887	1.00 67.85
	MOTA	1486	CB	LYS A	180	44.431	7.615	15.360	1.00 69.83
	MOTA	1487	CG	LYS A		45.938	7.673	15.581	1.00 73.65
25	ATOM	1488	CD	LYS A		46.681	8.326	14.427	1.00 76.04
25	MOTA	1489	CE	LYS A		48.016	8.889	14.887	1.00 75.99
	ATOM	1490	NZ	LYS A		47.829	10.056	15.790	1.00 78.28 1.00 66.93
	ATOM ATOM	1491 1492	N CA	ASN A		43.017 43.126	10.216 11.609	16.652 17.113	1.00 66.52
	ATOM	1493	C	ASN A		42.128	11.842	18.240	1.00 65.58
30	ATOM	1494	ŏ	ASN A		41.133	11.131	18.348	1.00 65.86
	ATOM	1495	CB	ASN A		43.174	12.454	16.113	0.00 99.00
	ATOM	1496	CG	ASN A		44.528	12.902	15.624	0.00 99.00
	ATOM	1497	OD1	ASN A	181	45.545	12.248	15.833	0.00 99.00
	MOTA	1498	ND2	ASN A	181	44.525	14.056	14.935	0.00 99.00
35	ATOM	1499	N	LYS A		42.432	12.756	19.155	1.00 65.06
	MOTA	1500	CA	LYS A		41.483	13.086	20.232	1.00 62.47
	ATOM	1501	C	LYS A		40.755	14.370	19.855	1.00 60.44
	ATOM	1502 1503	0	LYS A		40.951 42.257	15.405 13.224	20.491 21.544	1.00 60.89 1.00 68.03
40	ATOM ATOM	1504	CB CG	LYS A		41.462	13.626	22.774	1.00 70.69
.0	ATOM	1505	CD	LYS A		42.223	14.606	23.651	1.00 73.12
	ATOM	1506	CE	LYS A		41.360	15.246	24.718	1.00 73.28
	ATOM	1507	NZ	LYS A		40.729	16.534	24.325	1.00 74.63
	ATOM	1508	N	VAL A	183	40.007	14.401	18.761	1.00 58.04
45	ATOM	1509	CA	VAL A	183	39.240	15.559	18.324	1.00 55.16
	ATOM	1510	С	VAL A		37.899	15.073	17.781	1.00 52.42
	MOTA	1511	0	VAL A		37.902	14.220	16.898	1.00 52.43
	ATOM	1512	CB	VAL A		39.936	16.462	17.302	1.00 58.84
50	MOTA	1513		VAL A		38.965	17.219	16.395	1.00 61.12
50	ATOM ATOM	1514 1515	N	VAL A		40.809 36.785	17.504 15.581	18.010 18.302	1.00 60.87 1.00 49.48
	ATOM	1516	CA	TRP A			15.042	17.878	1.00 45.59
	MOTA	1517	C	TRP A			16.159	17.706	1.00 44.01
	ATOM	1518		TRP A			17.353	17.913	1.00 42.88
55	MOTA	1519		TRP A			13.926	18.839	1.00 42.62
	MOTA	1520	CG	TRP A			14.460	20.253	1.00 39.47
	MOTA	1521					15.236	20.830	1.00 37.50
	MOTA	1522		TRP A			14.271	21.216	1.00 41.84
60	ATOM	1523		TRP A			15.541	22.123	1.00 36.00
60	ATOM	1524		TRP A			14.963	22.380	1.00 39.37
	ATOM ATOM	1525 1526		TRP A			13.587	21.201 23.529	1.00 39.30 1.00~41.08
	ATOM	1526		TRP A			14.983 13.599	22.341	1.00 41.08
		,				53.200			

ATOM 1528 CHZ TRP A 184 37,692 14,293 23,486 1,00 42.374 ATOM 1529 N GUD A 185 32.291 15.809 17.270 1.00 42.374 ATOM 1529 N GUD A 185 32.291 16.770 17.099 1.00 42.374 ATOM 1521 C GLU A 185 32.211 16.770 17.099 1.00 42.70 ATOM 1522 O GLU A 185 30.590 15.062 17.506 1.00 43.74 ATOM 1534 CG GLU A 185 30.589 15.062 17.506 1.00 43.74 ATOM 1535 CD GUD A 185 30.589 15.062 17.506 1.00 43.74 ATOM 1535 CD GUD A 185 31.093 17.074 15.635 1.00 42.10 ATOM 1535 CD GUD A 185 31.093 17.074 15.635 1.00 42.10 ATOM 1535 CD GUD A 185 31.953 17.527 12.910 1.00 40.53 ATOM 1536 ORI GUD A 185 31.953 17.527 12.910 1.00 40.53 ATOM 1538 N VAL A 186 30.374 17.021 18.653 1.00 42.12 ATOM 1539 CA VAL A 186 27.943 17.055 18.053 1.00 43.51 ATOM 1540 C VAL A 186 27.943 17.105 18.653 1.00 43.51 ATOM 1540 C VAL A 186 27.943 17.105 18.653 1.00 43.51 ATOM 1541 CO VAL A 186 29.339 17.008 20.872 1.00 41.67 ATOM 1544 CG2 VAL A 186 29.339 17.008 20.872 1.00 41.67 ATOM 1546 CA HIS A 1867 27.012 16.272 18.454 1.00 46.52 ATOM 1546 CA HIS A 187 25.679 16.556 18.003 1.00 33.95 ATOM 1546 CA HIS A 187 25.679 16.556 18.003 1.00 50.055 ATOM 1547 CHIS A 187 24.447 15.055 19.262 1.00 51.22 ATOM 1548 O HIS A 187 24.447 15.055 19.262 1.00 51.22 ATOM 1548 O HIS A 187 24.447 15.055 19.262 1.00 51.22 ATOM 1545 NEL HIS A 187 24.447 15.055 19.262 1.00 51.22 ATOM 1554 NEZ HIS A 187 24.447 15.055 19.262 1.00 51.22 ATOM 1555 CD HIS A 187 25.679 16.656 18.003 1.00 50.55 1.22 ATOM 1555 CD HIS A 187 25.679 18.656 18.003 1.00 50.55 1.22 ATOM 1556 CG HIS A 187 25.679 18.656 18.003 1.00 50.55 1.22 ATOM 1556 CG HIS A 187 25.679 18.656 18.003 1.00 50.05 1.22 ATOM 1556 CG HIS A 187 25.679 18.656 18.003 1.00 50.05 1.22 ATOM 1556 CG HIS A 187 25.679 18.656 18.003 1.00 50.05 1.22 ATOM 1556 CG HIS A 187 25.679 18.656 18.003 1.00 50.05 1.22 ATOM 1556 CG HIS A 187 25.679 18.684 18.004 18.00 50.05 18.22 ATOM 1556 CG HIS A 187 25.679 18.684 18.00 60.00 50.05 18.22 ATOM 1557 NEZ HIS A 187 25.679 18.884 18.00 60.00 50.05 18.22 ATOM 1557 NEZ HIS A 187 25.250 18.384 18.00 60.00 50.05 18.22 ATOM										
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ATOM 1.530 CA GLU A 185 32.211 16.770 17.099 1.00 42.70 ATOM 1531 C GLU A 185 30.950 16.204 17.765 1.00 43.74 ATOM 1532 C GLU A 185 30.950 16.002 17.506 1.00 43.74 ATOM 1533 C GLU A 185 30.589 15.062 17.506 1.00 43.74 ATOM 1534 CG GLU A 185 31.903 17.074 15.635 1.00 42.03 ATOM 1535 C GLU A 185 33.023 17.900 14.999 1.00 38.91 ATOM 1536 OE1 GLU A 185 31.903 17.527 12.910 1.00 40.53 ATOM 1537 C BU A 185 31.953 17.527 12.910 1.00 40.53 ATOM 1538 N VAL A 186 30.374 17.021 18.653 1.00 43.76 ATOM 1540 C VAL A 186 30.374 17.021 18.653 1.00 43.76 ATOM 1540 C VAL A 186 27.943 17.165 18.791 1.00 45.37 ATOM 1540 C VAL A 186 29.339 17.008 20.872 1.00 41.67 ATOM 1544 CG2 VAL A 186 29.339 17.008 20.872 1.00 41.67 ATOM 1546 CA HIS A 186 30.697 16.596 21.452 1.00 34.96 ATOM 1546 CA HIS A 187 25.679 16.656 18.003 34.09 ATOM 1546 CA HIS A 187 25.679 16.656 18.003 34.09 ATOM 1546 CA HIS A 187 25.679 16.656 18.003 1.00 50.05 ATOM 1547 C HIS A 187 24.447 15.055 19.262 1.00 52.23 ATOM 1548 C BHIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1549 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CG HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 22.833 15.710 15.495 10.00 54.05 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 55.223 ATOM 1550 CB HIS A 189 22.833 16.882 20.591 1.00 56.05 ATOM 1550 CB ALA A 188 22.883 16.882 20.591 1.00 56.05 ATOM 1556 CA ALA A 188 22.883 16.882 10.93 1.00 56.05 ATOM 1556 CA ALA A 188 22.883 16.882 10.93 1.00 56.05 ATOM 1566 C C GLY A 189 19.802 1.107 17.773 19.155 1.00 66.864 ATOM 1568 C C GLY A 189 19.25.450 22.451 17.660 1.00 68.85 ATOM 1568 C C GLY A 189 19										
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ATOM 1544 CG2 VAL A 186	15	ATOM	1542	CB	VAL A	186			-	
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ATOM 1546 CA HIS A 187 25.679 16.656 18.003 1.00 50.055 ATOM 1548 C HIS A 187 24.620 16.257 19.023 1.00 52.23 ATOM 1548 C HIS A 187 24.447 15.055 19.262 1.00 52.60 ATOM 1549 CB HIS A 187 25.329 15.949 16.672 1.00 51.22 ATOM 1550 CG HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1551 ND1 HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1552 CD2 HIS A 187 27.633 15.710 15.455 1.00 54.05 ATOM 1553 CE1 HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1553 CE1 HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1553 NALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1555 N ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1556 CA ALA A 188 22.883 16.882 20.591 1.00 57.90 ATOM 1558 O ALA A 188 20.747 17.673 21.356 1.00 60.86 ATOM 1558 O ALA A 188 21.502 17.477 20.393 1.00 59.90 ATOM 1550 N GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1560 C GLY A 189 19.809 18.381 18.867 1.00 62.76 ATOM 1565 CA GLY A 189 19.809 18.381 18.867 1.00 62.76 ATOM 1566 CA GLY A 189 19.802 18.381 18.867 1.00 62.76 ATOM 1566 CA GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 CA GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 CA GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1567 C GLN A 191 23.029 21.274 16.698 1.00 58.39 ATOM 1567 C GLN A 191 23.029 21.274 16.698 1.00 58.39 ATOM 1567 C GLN A 191 23.029 21.274 16.698 1.00 58.39 ATOM 1567 C GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1567 C GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1567 C GLN A 191 24.972 24.927 17.760 1.00 52.57 ATOM 1569 CA GLN A 191 24.972 24.927 17.760 1.00 52.59 ATOM 1570 C GLN A 191 24.972 24.927 17.760 1.00 52.59 ATOM 1570 C GLN A 191 24.972 24.927 17.760 1.00 52.59 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.59 ATOM 1570 C GLN A 191 26.437 25.200 17.50 1.00 59.90 ATOM 1570 C GLN A 191 26.467 27.43 18.451 1.00 99.00 ATOM 1570 C GLN A 191 26.467 27.43 18.451 1.00 59.90 ATOM 1570 C GLN A 191 26.467 27.43 18.451 1.00 59.90 ATOM 1570 C GLN A 191 26.470 27.24 1.00 1.00 58.35 ATOM 1580 C GLN A 191 26.470 27.24 1.00 1.00 58.35 ATOM 1580 C GLN A 191 26.470 27.24 1.00		ATOM	1544	CG2	VAL A	186	30.697			
20 ATOM 1546 CA HIS A 187 25.679 16.656 18.003 1.00 50.052.23 ATOM 1548 0 HIS A 187 24.447 15.055 19.262 1.00 52.23 ATOM 1550 CB HIS A 187 25.329 15.949 16.672 1.00 52.60 ATOM 1550 CG HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1555 CD2 HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1555 CD2 HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1555 CD2 HIS A 187 27.333 15.710 15.495 1.00 54.05 ATOM 1555 CD2 HIS A 187 27.333 15.710 15.495 1.00 54.05 ATOM 1555 N ALA A 188 23.836 17.199 19.524 1.00 54.05 ATOM 1555 N ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1555 N ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1555 CA ALA A 188 22.883 16.882 20.551 1.00 57.60 ATOM 1555 C ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1555 CA ALA A 188 23.836 17.199 19.524 1.00 59.90 ATOM 1556 CA ALA A 188 23.836 17.199 19.524 1.00 59.90 ATOM 1556 CA ALA A 188 23.836 17.199 19.524 1.00 59.90 ATOM 1556 CA ALA A 188 23.501 17.291 21.292 1.00 57.50 ATOM 1560 N GLY A 189 19.809 18.381 18.867 1.00 60.86 ATOM 1563 C C GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1564 N GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1565 CA GLY A 189 19.802 18.381 18.809 1.00 63.40 ATOM 1566 CA GLY A 190 21.051 20.429 18.488 1.00 62.37 ATOM 1566 CA GLY A 190 21.051 20.429 18.488 1.00 62.37 ATOM 1566 CA GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1567 C GLY A 190 23.029 21.274 16.698 1.00 58.39 ATOM 1567 C GLY A 190 23.029 21.274 16.698 1.00 58.39 ATOM 1568 CA GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 24.466 23.574 ATOM 1570 C GLN A 191 24.466 23.574 ATOM 1570 C GLN A 191 24.466 23.77 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.67 ATOM 1570 C GLN A 191 24.466 23.77 ATOM 1570 C GLN A 191 24.466		ATOM	1545	N	HIS A	187	27.012	16.272		
20 ATOM 1548 C HIS A 187 24.620 16.257 19.023 1.00 52.23 ATOM 1548 CB HIS A 187 25.329 15.949 16.672 1.00 52.60 ATOM 1550 CB HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1551 ND1 HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1551 ND1 HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1552 CD2 HIS A 187 26.356 16.159 15.600 1.00 55.72 ATOM 1553 CE1 HIS A 187 27.216 16.916 14.467 1.00 54.05 ATOM 1554 NE2 HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1555 NALA A 188 23.836 17.199 19.524 1.00 54.65 ATOM 1556 CA ALA A 188 22.883 16.882 20.591 1.00 57.68 ATOM 1555 C ALA A 188 22.883 16.882 20.591 1.00 57.68 ATOM 1559 CB ALA A 188 21.502 17.477 20.393 1.00 59.90 ATOM 1556 CA ALA A 188 23.501 17.291 21.929 1.00 57.50 ATOM 1561 CA GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1563 C GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1564 N GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1566 C GLY A 189 19.862 19.892 18.710 1.00 62.45 ATOM 1566 C GLY A 189 19.862 19.892 18.710 1.00 62.45 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1567 CA GLN A 191 23.132 22.853 1.00 59.00 ATOM 1567 CA GLN A 191 23.132 22.853 1.00 56.77 ATOM 1567 CA GLN A 191 23.132 22.853 1.00 56.77 ATOM 1570 C GLN A 191 23.132 22.853 17.83 1.00 56.67 ATOM 1570 C GLN A 191 25.462 22.451 17.660 1.00 58.39 ATOM 1573 CG GLN A 191 25.462 22.451 17.660 1.00 58.39 ATOM 1573 CG GLN A 191 25.462 22.451 17.660 1.00 59.00 ATOM 1576 CA GLN A 191 25.462 22.451 17.667 1.00 52.57 ATOM 1577 CA GLN A 191 25.462 22.451 17.667 1.00 52.57 ATOM 1577 CA GLN A 191 25.462 22.451 17.667 1.00 52.57 ATOM 1577 CA GLN A 191 25.462 22.451 17.667 1.00 52.57 ATOM 1578 CA VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1588 CB CB CLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1578 CA VAL A 192 27.666 26.948 17.561 0.00 99.00 ATOM 1578 CA VAL A 192 27.660 1.00 2.771 15.544 1.00 49.84 ATOM 1588 CB ILE A 193 28.831 20			1546	CA	HIS A	187	25.679	16.656	18.003	
ATOM 1548 6 HIS A 187 24.447 15.055 19.262 1.00 52.60 ATOM 1550 CG HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1551 DI HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1552 CD2 HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1552 CD2 HIS A 187 26.335 16.916 14.467 1.00 55.72 ATOM 1555 CD2 HIS A 187 27.633 15.710 15.455 1.00 54.05 ATOM 1555 NA ALA A 188 27.216 16.925 13.713 1.00 49.24 ATOM 1555 NA ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1555 CC A ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1555 CB ALA A 188 21.502 17.477 20.393 1.00 59.90 ATOM 1555 CB ALA A 188 20.747 17.673 21.356 1.00 60.66 ATOM 1555 CB ALA A 188 23.501 17.291 21.929 1.00 57.50 ATOM 1560 N GLY A 189 21.107 17.773 19.155 1.00 61.42 ATOM 1561 CA GLY A 189 19.862 19.892 18.710 1.00 62.45 ATOM 1563 C GLY A 189 19.862 19.892 18.70 1.00 62.45 ATOM 1566 CA GLY A 189 19.862 19.892 18.70 1.00 62.45 ATOM 1566 CA GLY A 189 19.862 19.892 18.70 1.00 62.37 ATOM 1566 CA GLY A 190 21.051 20.429 18.48 1.00 62.37 ATOM 1566 CA GLY A 190 21.051 20.429 18.48 1.00 62.37 ATOM 1566 CA GLY A 190 21.051 20.429 18.48 1.00 62.37 ATOM 1566 CA GLY A 190 21.051 20.429 18.48 1.00 62.37 ATOM 1566 CA GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1567 C GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1570 C GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1571 C GLN A 191 24.477 25.200 17.501 1.00 52.69 ATOM 1572 CB GLN A 191 24.477 25.200 17.502 17.501 1.00 52.69 ATOM 1577 CD GLN A 191 24.477 25.200 17.502 17.502 17.502 ATOM 1578 CB GLN A 191 24.477 25.200 17.502 17.502 17.502 ATOM 1578 CB GLN A 191 24.477 25.200 17.502 17.502 17.502 17.503 ATOM 1578 CB GLN A 191 24.477 25.200 17.502 17.502 17.502 17.500 ATOM 1577 CD GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1577 CD GLN A 191 25.459 27.683 16.891 0.00 49.07 ATOM 1578 CB GLN A 191 26.457 72.403 18.451 0.00 45.59 ATOM 1578 CB GLN A 191 27.902 27.914 17.966 15.544 1.00 42.50 ATOM 1588 CB CB ILE A 193 31.569 19.822 19.009 1.00 44.47 ATOM 1588 CB LE A 193 31.569 19.	20			С			24.620	16.257		1.00 52.23
ATOM 1549 CB HIS A 187 25.329 15.949 16.672 1.00 53.27 ATOM 1551 ND1 HIS A 187 26.356 16.916 14.467 1.00 55.72 ATOM 1552 CD2 HIS A 187 27.633 15.710 15.495 1.00 54.05 ATOM 1553 CE1 HIS A 187 27.633 15.710 15.495 1.00 54.05 ATOM 1555 ND1 HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1555 ND2 HIS A 187 28.134 16.205 14.329 1.00 53.78 ATOM 1556 CA ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1556 CA ALA A 188 22.883 16.882 20.591 1.00 57.68 ATOM 1557 C ALA A 188 21.502 17.477 20.393 1.00 59.90 ATOM 1558 O ALA A 188 21.502 17.477 20.393 1.00 59.90 ATOM 1558 O ALA A 188 21.502 17.477 20.393 1.00 59.90 ATOM 1556 CB ALA A 188 23.501 17.291 21.929 1.00 57.50 ATOM 1561 CA GLY A 189 21.107 17.773 19.155 1.00 61.42 ATOM 1562 C GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1563 O GLY A 189 19.862 19.892 18.710 1.00 62.76 ATOM 1566 C GLY A 189 19.862 19.892 18.700 1.00 63.40 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1568 N GLN A 191 23.029 21.274 16.958 1.00 56.77 ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1570 C GLN A 191 25.462 22.451 17.660 1.00 58.39 ATOM 1571 O GLN A 191 25.462 22.451 17.561 1.00 52.69 ATOM 1573 CG GLN A 191 25.462 22.451 17.567 1.00 52.57 ATOM 1576 NEZ GLN A 191 25.462 22.451 17.567 1.00 62.97 ATOM 1577 N VALA 192 26.162 22.451 17.567 1.00 62.97 ATOM 1578 CG GLN A 191 25.462 22.451 17.561 0.00 99.00 ATOM 1576 NEZ GLN A 191 25.462 22.451 17.561 0.00 99.00 ATOM 1577 N VALA 192 27.960 20.717 15.544 1.00 45.59 ATOM 1578 CG VAL A 192 28.237 21.647 17.551 1.00 44.77 ATOM 1578 CG GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1578 CA LA A 192 28.237 21.647 17.875 1.00 44.77 ATOM 1580 CG UNLA 192 28.237 21.647 17.875 1.00 44.77 ATOM 1581 CB VAL A 192 27.960 20.717 15.5544 1.00 49.07 ATOM 1588 CG UNLA 192 28.831 29.882 18.775 1.00 44.79 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.00 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.00 ATOM 1588 CB ILE A 193 31.569 19.822 19.0				,	HIS A	187	24.447	15.055	19.262	
ATOM 1550 CG HIS A 187 26.356 16.159 15.600 1.00 53.27 ATOM 1551 ND1 HIS A 187 26.135 16.916 14.467 1.00 55.72 ATOM 1552 CD2 HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1553 CE1 HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1555 N NALA A 188 23.836 17.199 19.524 1.00 53.78 ATOM 1555 CA ALA A 188 22.883 16.882 20.591 1.00 57.68 ATOM 1557 C ALA A 188 22.883 16.882 20.591 1.00 57.68 ATOM 1556 CA ALA A 188 21.502 17.477 20.393 1.00 59.90 ATOM 1556 N ALA A 188 23.501 17.291 21.325 1.00 60.86 ATOM 1550 N GLY A 189 21.107 17.773 19.155 1.00 61.42 ATOM 1560 N GLY A 189 21.107 17.773 19.155 1.00 62.45 ATOM 1560 N GLY A 189 19.802 18.881 18.867 1.00 62.45 ATOM 1562 C GLY A 189 19.802 18.881 18.807 1.00 62.45 ATOM 1565 CA GLY A 189 19.802 18.881 18.807 1.00 62.45 ATOM 1565 CA GLY A 189 19.802 18.892 18.710 1.00 62.45 ATOM 1565 CA GLY A 189 19.802 18.892 18.710 1.00 62.45 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1567 N GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1567 N GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1567 N GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1567 N GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1567 N GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1567 N GLY A 191 23.173 23.285 17.983 1.00 54.69 ATOM 1570 C GLN A 191 23.173 23.285 17.983 1.00 54.69 ATOM 1570 C GLN A 191 23.173 23.285 17.983 1.00 54.69 ATOM 1573 CG GLN A 191 24.466 23.554 17.502 1.00 62.97 ATOM 1575 OCI GLN A 191 26.462 22.451 17.760 1.00 58.35 ATOM 1578 CG GLN A 191 26.462 22.451 17.601 1.00 58.35 ATOM 1578 CG GLN A 191 26.462 22.451 17.760 1.00 58.35 ATOM 1578 CG GLN A 191 26.462 22.451 17.760 1.00 58.35 ATOM 1578 CG GLN A 191 26.462 22.451 17.760 1.00 59.00 ATOM 1578 CG GLN A 191 26.462 22.451 17.760 1.00 59.00 ATOM 1578 CG GLN A 191 26.462 22.451 17.760 1.00 54.59 ATOM 1578 CG GLN A 191 26.462 22.451 17.760 1.00 54.59 ATOM 1578 CG GLN A 191 26.462 22.451 17.760 1.00 54.59 ATOM 1578 CG GLN A 191 2							25.329	15.949	16.672	1.00 51.22
25 ATOM 1551 ND1 HIS A 187 27.633 15.710 15.495 1.00 54.05 ATOM 1553 CEI HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1555 N NE2 HIS A 187 27.216 16.925 13.713 1.00 49.24 ATOM 1555 N NE2 HIS A 188 23.836 17.199 19.524 1.00 53.78 ATOM 1555 N ALA A 188 23.836 17.199 19.524 1.00 54.61 ATOM 1556 CA ALA A 188 22.883 16.882 20.591 1.00 57.68 ATOM 1557 C ALA A 188 22.883 16.882 20.591 1.00 57.68 ATOM 1558 O ALA A 188 20.747 17.673 21.356 1.00 60.86 ATOM 1556 CB ALA A 188 23.501 17.291 21.929 1.00 57.50 ATOM 1556 CB ALA A 188 23.501 17.291 21.929 1.00 57.50 ATOM 1560 N GLY A 189 21.107 17.773 19.155 1.00 61.42 ATOM 1561 CA GLY A 189 19.809 18.381 18.867 1.00 62.45 ATOM 1563 O GLY A 189 19.862 19.892 18.710 1.00 62.45 ATOM 1563 O GLY A 189 18.863 20.613 18.809 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 62.37 ATOM 1566 C GLY A 190 21.051 20.429 18.448 1.00 60.60 ATOM 1566 C GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1570 C GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1571 O GLN A 191 22.466 22.451 17.687 1.00 52.57 ATOM 1573 CG GLN A 191 22.466 22.451 17.687 1.00 52.57 ATOM 1576 NE2 GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1576 NE2 GLN A 191 26.462 22.451 17.687 1.00 52.57 ATOM 1576 NE2 GLN A 191 26.462 22.451 17.687 1.00 52.57 ATOM 1577 N VALA A 192 27.960 20.717 7.502 1.00 69.00 ATOM 1576 NE2 GLN A 191 26.462 22.451 17.502 1.00 69.00 ATOM 1576 NE2 GLN A 191 26.462 22.451 17.504 1.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VALA 192 27.960 20.717 7.554 1.00 44.47 ATOM 1580 CG UNLA 192 28.473 22.853 17.803 1.00 45.59 ATOM 1581 CB VALA 192 27.960 20.717 7.554 1.00 49.07 ATOM 1585 CA LLE A 193 31.266 21.002 19.00 45.59 ATOM 1588 CB LLE A 193 31.266 21.009 19.127 1.00 40.00 40.84 ATOM 1588 CB LLE A 193 31.266 21.009 19.127 1.00 40.00 38.85 ATOM 1588 CB LLE A 193 31.266 21.009 19.127 1.00 40.00 38.85 A							26.356	16.159	15.600	1.00 53.27
25								16.916	14.467	1.00 55.72
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ATOM 1565 CA GLY A 190 21.211 21.883 18.338 1.00 60.60 ATOM 1566 C GLY A 190 22.551 22.159 17.660 1.00 58.62 ATOM 1567 O GLY A 190 23.029 21.274 16.958 1.00 58.39 ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1569 CA GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 ATOM 1573 CG GLN A 191 24.972 24.927 17.760 1.00 58.35 ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1575 OE1 GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1578 CA VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 CG VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 CG VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 31.569 19.822 19.009 1.00 40.00 ATOM 1585 CA ILE A 193 31.569 19.822 19.009 1.00 40.00 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.00 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.00 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.00 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 38.63		MOTA	1563	0	GLY A	189				
ATOM 1566 C GLY A 190 22.551 22.159 17.660 1.00 58.62 40 ATOM 1567 O GLY A 190 23.029 21.274 16.958 1.00 58.39 ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1569 CA GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 ATOM 1572 CB GLN A 191 24.972 24.927 17.760 1.00 58.39 ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1575 OE1 GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 18.451 0.00 99.00 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1581 CB VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1588 CB ILE A 193 31.246 21.009 19.127 1.00 40.01 ATOM 1588 CB ILE A 193 31.246 21.009 19.127 1.00 40.02 ATOM 1588 CB ILE A 193 31.246 21.009 19.127 1.00 40.02 ATOM 1588 CB ILE A 193 31.246 21.009 19.127 1.00 40.02 ATOM 1588 CB ILE A 193 31.246 21.009 19.127 1.00 40.02		ATOM	1564	N						
40 ATOM 1567 O GLY A 190 23.029 21.274 16.958 1.00 58.39 ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1569 CA GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 ATOM 1572 CB GLN A 191 24.972 24.927 17.760 1.00 58.35 ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1574 CD GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1578 CA VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1579 C VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 C VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1588 CB ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 38.63		ATOM	1565	CA	GLY A	190				
ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1569 CA GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 45 ATOM 1572 CB GLN A 191 24.972 24.927 17.760 1.00 58.35 ATOM 1573 CG GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 55 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 40.84 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1587 O ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 38.63		MOTA	1566	С	GLY A	190	22.551			
ATOM 1568 N GLN A 191 23.173 23.285 17.983 1.00 56.77 ATOM 1569 CA GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 ATOM 1572 CB GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1574 CD GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 55 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1586 C ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1587 O ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1588 CB ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 38.63	40	MOTA	1567	0	GLY A	190	23.029			
ATOM 1569 CA GLN A 191 24.466 23.554 17.336 1.00 54.69 ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 ATOM 1573 CG GLN A 191 24.972 24.927 17.760 1.00 62.97 ATOM 1573 CG GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1582 CG1 VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 40.84 ATOM 1586 C ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 38.63 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 38.63 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 38.63			1568	N	GLN A	191	23.173	23.285		
ATOM 1570 C GLN A 191 25.462 22.451 17.687 1.00 52.57 ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 45 ATOM 1572 CB GLN A 191 24.972 24.927 17.760 1.00 58.35 ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1574 CD GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1579 C VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 CG VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 40.84 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 38.63				CA	GLN A	191	24.466	23.554	17.336	
ATOM 1571 O GLN A 191 25.599 22.082 18.858 1.00 52.69 ATOM 1572 CB GLN A 191 24.972 24.927 17.760 1.00 58.35 ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1574 CD GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1581 CB VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1582 CG1 VAL A 192 27.960 20.717 15.544 1.00 39.90 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1584 N ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1585 CA ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1588 CB ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 29.715 20.868 21.104 1.00 36.14				С	GLN A	191	25.462	22.451	17.687	
45 ATOM 1572 CB GLN A 191 24.972 24.927 17.760 1.00 58.35 ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1574 CD GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1587 O ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63							25.599	22.082		
ATOM 1573 CG GLN A 191 26.437 25.200 17.502 1.00 62.97 ATOM 1574 CD GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 26.874 20.237 14.584 1.00 40.84 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1587 O ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63	45						24.972	24.927	17.760	1.00 58.35
ATOM 1574 CD GLN A 191 26.166 26.948 17.561 0.00 99.00 ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1581 CB VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1582 CG1 VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 26.874 20.237 14.584 1.00 40.84 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1586 C ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1588 CB ILE A 193 29.875 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63							26.437	25.200	17.502	1.00 62.97
ATOM 1575 OE1 GLN A 191 25.459 27.683 16.891 0.00 99.00 ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 50 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 26.874 20.237 14.584 1.00 40.84 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63							26.166	26.948	17.561	0.00 99.00
ATOM 1576 NE2 GLN A 191 27.070 27.403 18.451 0.00 99.00 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1583 CG2 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1587 O ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63									16.891	0.00 99.00
50 ATOM 1577 N VAL A 192 26.162 21.943 16.684 1.00 49.07 ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 55 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 26.874 20.237 14.584 1.00 40.84 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1587 O ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63				_						0.00 99.00
ATOM 1578 CA VAL A 192 27.264 21.012 16.898 1.00 45.59 ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 26.874 20.237 14.584 1.00 40.84 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 ATOM 1587 O ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63	50									1.00 49.07
ATOM 1579 C VAL A 192 28.237 21.647 17.875 1.00 44.47 ATOM 1580 O VAL A 192 28.473 22.853 17.803 1.00 45.15 ATOM 1581 CB VAL A 192 27.960 20.717 15.544 1.00 42.50 55 ATOM 1582 CG1 VAL A 192 29.047 19.665 15.684 1.00 39.90 ATOM 1583 CG2 VAL A 192 26.874 20.237 14.584 1.00 40.84 ATOM 1584 N ILE A 193 28.831 20.882 18.775 1.00 41.81 ATOM 1585 CA ILE A 193 29.875 21.406 19.636 1.00 39.71 ATOM 1586 C ILE A 193 31.246 21.009 19.127 1.00 40.00 60 ATOM 1587 O ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63	30									
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60 ATOM 1587 O ILE A 193 31.569 19.822 19.009 1.00 40.12 ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63		MOTA	1586	С						
ATOM 1588 CB ILE A 193 29.715 20.868 21.104 1.00 36.14 ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63	60	ATOM	1587	0						
ATOM 1589 CG1 ILE A 193 28.303 21.218 21.573 1.00 38.63				CB						
				CG1						
				CG2	ILE A	193	30.765	21.585	21.957	1.00 38.85

							00 501	00 000	1 00 41 20
	MOTA	1591		ILE A		27.916		22.922	1.00 41.29
	ATOM	1592	N	LEU A		32.075		18.852	1.00 39.67
	ATOM	1593	CA	LEU A		33.436		18.388	1.00 40.23
_	MOTA	1594	С	LEU A		34.455		19.486	1.00 40.97
5	MOTA	1595	0	LEU A		34.136		20.557	1.00 40.07
	ATOM	1596	CB	LEU A		33.741	22.794	17.252	1.00 38.19
	MOTA	1597	CG	LEU A	194	32.736		16.101	1.00 42.91
	MOTA	1598		LEU A		33.203	23.702	14.980	1.00 42.33
	MOTA	1599	CD2	LEU A	194	32.593	21.362	15.514	1.00 41.05
10	ATOM	1600	N	CYS A	195	35.658	21.430	19.269	1.00 41.29
	MOTA	1601	CA	CYS A	195	36.711	21.575	20.273	1.00 43.15
	MOTA	1602	С	CYS A	195	36.956	23.045	20.562	1.00 45.32
	ATOM	1603	0	CYS A	195	37.083	23.872	19.671	1.00 44.47
	ATOM	1604	СВ	CYS A		37.981	20.893	19.785	1.00 44.75
15	ATOM	1605	SG	CYS A		39.358	21.057	20.920	1.00 43.19
1.5	ATOM	1606	N	PRO A		36.918	23.423	21.847	1.00 46.44
	ATOM	1607	CA	PRO A		36.978	24.814	22.245	1.00 47.49
	ATOM	1608	C	PRO A		38.376	25.335	22.514	1.00 48.05
	ATOM	1609	Õ	PRO A		38.575	26.531	22.759	1.00 49.91
20	MOTA	1610	СВ	PRO A		36.123	24.820	23.515	1.00 48.09
20				PRO A		36.293	23.449	24.079	1.00 47.48
	MOTA	1611	CG				22.513	23.018	1.00 47.09
	ATOM	1612	CD	PRO A		36.834			1.00 47.03
	ATOM	1613	N	THR A		39.365	24.477	22.488	1.00 49.51
25	ATOM	1614	CA	THR A		40.753	24.821	22.766	
25	MOTA	1615	С	THR A		41.610	24.697	21.491	1.00 48.70
	MOTA	1616	0	THR A		41.132	24.143	20.508	1.00 47.51
	ATOM	1617	CB	THR A		41.337	23.819	23.789	1.00 54.19
	ATOM	1618	OG1			42.063	22.755	23.133	1.00 60.20
	MOTA	1619	CG2			40.249	23.146	24.620	1.00 60.00
30	ATOM	1620	N	SER A		42.874	25.104	21.600	1.00 48.43
	MOTA	1621	CA	SER A	198	43.755	25.011	20.443	1.00 49.41
	MOTA	1622	С	SER A	198	44.106	23.572	20.088	1.00 51.13
	ATOM	1623	0	SER A	198	44.340	22.748	20.974	1.00 50.32
	ATOM	1624	CB	SER A	198	45.022	25.837	20.600	1.00 41.67
35	ATOM	1625	OG	SER A	198	44.689	27.176	20.863	1.00 42.21
	ATOM	1626	N	VAL A	199	44.135	23.321	18.783	1.00 51.78
	ATOM	1627	CA	VAL A		44.448	22.018	18.210	1.00 54.21
	ATOM	1628	C	VAL A	199	45.846	22.063	17.593	1.00 55.85
	ATOM	1629	ō	VAL A		46.229	23.043	16.958	1.00 55.32
40	ATOM	1630	ČВ	VAL A		43.415	21.673	17.105	1.00 55.83
	ATOM	1631		VAL A		43.848	20.450	16.311	1.00 58.48
	ATOM	1632		VAL A		42.081	21.363	17.794	1.00 58.90
	ATOM	1633	N	PHE A		46.643	21.031	17.823	1.00 57.80
	ATOM	1634	CA	PHE A		48.033	20.977	17.458	1.00 60.84
45	ATOM	1635	C	PHE A		48.501	19.863	16.538	1.00 63.34
40	ATOM	1636	0	PHE A		47.988	18.771	16.373	1.00 63.71
	ATOM	1637	СВ	PHE A		48.976	20.962	18.695	1.00 56.48
			CG	PHE A		49.009	22.350	19.286	1.00 51.93
	ATOM	1638						18.779	1.00 50.53
50	ATOM	1639		PHE A		49.867	23.304 22.686	20.298	1.00 52.06
50	MOTA	1640		PHE A		48.118			1.00 32.00
	ATOM	1641		PHE A		49.844	24.596	19.289	
	ATOM	1642		PHE A		48.104	23.972	20.813	1.00 46.67
	MOTA	1643	CZ	PHE A		48.952	24.921	20.283	1.00 48.73
	ATOM	1644	N	SER A		49.612	20.201	15.906	1.00 65.54
55	MOTA	1645	CA	SER A		50.520	19.367	15.151	1.00 67.49
	MOTA	1646	C	SER A		50.543	17.927	15.652	1.00 68.56
	MOTA	1647	0	SER A		50.873	17.710	16.841	1.00 69.46
	MOTA	1648	CB	SER A			19.984	15.374	1.00 69.06
	ATOM	1649	OG	SER A		51.799	21.376	15.666	1.00 64.56
60	ATOM	1650	OT	SER A	201	50.201	17.025	14.856	1.00 71.71
	ATOM	1651	OWO	WAT W	1	16.850	8.350	41.749	1.00 33.70
	ATOM	1652	OWO	WAT W	2	14.700	3.706	36.739	1.00 34.70
	ATOM	1653	OWO	W TAW	3	23.512	-21.581	45.725	1.00 35.04

	ATOM	1654	OW0	WAT	W	4			-16.192	51.826	1.00	
	ATOM	1655	OWO	WAT	W	5		27.151	6.021	35.728	1.00	
	ATOM	1656	OWO	TAW	W	6		35.841	19.641	17.028	1.00	
	ATOM	1657	OW0	WAT	W	7		12.924	7.105	31.382		36.46
5.	ATOM	1658	OW0	WAT	W	8		22.396	20.058	35.878	1.00	
	ATOM	1659	OWO	WAT	W	9		17.562		44.759	1.00	
	ATOM	1660	OWO	WAT	W	10		23.931	7.992	29.610		38.55
	ATOM	1661	OWO	WAT	W	11		32.085	22.981	25.237		38.76
	MOTA	1662	OWO	WAT	W	12		18.237	6.493	43.333		38.96
10	ATOM	1663	OW0	WAT	W	13		19.973	21.293	36.711		38.84
	ATOM	1664	OWO	TAW	W	14		14.757	-3.264	32.978		39.29
	ATOM	1665	OW0	WAT	W	15		19.948	-2.552	48.084		39.94
	ATOM	1666	OW0	WAT	W	16		13.394	-3.627	35.420		40.05
	ATOM	1667	OW0	WAT	W	17		24.218	1.873	40.503		40.12
15	ATOM	1668	OWO	WAT	W	18		12.970	-9.846	41.166		40.24
	ATOM	1669	OW0	WAT	W	19		29.332	23.835	36.728		40.10
	ATOM	1670	OW0	WAT	W	20		32.982	14.615	37.196		40.03
	ATOM	1671	OWO	WAT	W	21		15.963	-14.411	41.801		40.85
	ATOM	1672	OW0	TAW	W	22		36.115	14.124	27.538		41.62
20	ATOM	1673	OW0	TAW	W	23		36.759	24.316	27.854		41.58
	ATOM	1674	OW0	WAT	W	24		24.232	-12.120	40.700		41.18
	ATOM	1675	OWO	WAT	W	25		20.170	8.808	43.184		41.55
	ATOM	1676	OWO	WAT	W	26		14.174	8.391	52.525		43.14
	ATOM	1677	OWO	WAT	W	27		25.412	3.713	30.549		41.48
25	ATOM	1678		WAT		28		14.723	-7.678	41.271		41.77
	ATOM	1679		WAT		29		19.317	13.171	52.356		41.81
	ATOM	1680	OWO	WAT	W	30		23.266	21.233	27.612		42.08
	ATOM	1681	OWO	WAT	W	31		11.768	12.568	50.507		42.04
	ATOM	1682	OWO	WAT	W	32		13.539	-13.131	41.639		42.18
30	ATOM	1683		WAT		33		11.508	10.524	52.379		42.93
	ATOM	1684	OW0	WAT	W	34	`	3.363	-0.753	38.246		42.96
	MOTA	1685	OWO	WAT	W	35		22.835	-3.224	40.382		43.01
	ATOM	1686		TAW		36		26.824	22.825	28.526		43.00
	ATOM	1687	OW0	WAT	W	37		18.644	-1.265	41.392		43.97
35	ATOM	1688	OM0	WAT	W	38		8.736	-6.966	49.493		43.69
	ATOM	1689	OW0	WAT	W	39		15.651	-14.676	38.985		43.87
	ATOM	1690	OW0	WAT	W	40		8.333	-12.297	37.586		44.06
	ATOM	1691	OW0	WAT	W	41		25.939	7.843	39.161		44.11
	ATOM	1692	OWO	WAT	W	42		10.384	9.683	30.485		44.27
40	MOTA	1693	OW0	WAT	W	43		0.943	8.083	43.152		44.34
	ATOM	1694	OWO	WAT	W	44		21.071	2.692	43.998		44.65
	ATOM	1695	OW0	TAW	W	45		16.203	7.540	48.658		44.83
	ATOM	1696	OW0	WAT	W	46		21.491	-11.431	40.332		44.88
	ATOM	1697	OW0	WAT	W	47		21.292	-1.593	41.871	-	45.24
45	MOTA	1698		WAT		48		33.051	8.145	30.148	1.00	
-	ATOM	1699	OWO	WAT	W	49		11.644	15.303	50.268	1.00	
	ATOM	1700	OW0	WAT	W	50		35.864	19.699	14.264	1.00	
	ATOM	1701	OW0	WAT	W	51		7.067	6.695	50.824		46.58
	MOTA	1702	OW0	TAW	W	52		27.033	16.432	44.207	1.00	47.45
50	MOTA	1703	OWO	WAT	W	53		12.107	-10.902	38.882		47.44
	MOTA	1704	OWO	WAT	W	54		31.232	24.588	19.293		47.66
	ATOM	1705	OWO	TAW	W	55		21.781	-3.130	44.031		47.48
	MOTA	1706	OWO	WAT	W	56		7.169	-27.314	41.711	1.00	48.17
	MOTA	1707		WAT		57		33.861	-1.778	23.374		48.53
55	MOTA	1708		WAT		58		33.357	8.082	26.362		48.51
	ATOM	1709		WAT		59		26.396	24.163	13.998		49.70
	ATOM	1710		WAT		60		21,233	20.044	43.429		49.73
	ATOM	1711	OWO	WAT	W	61		39.604	24.739	18.318		49.28
	ATOM	1712		WAT		62		24.974	-18.827	45.601		50.87
60	ATOM	1713		WAT		63		21.207	-0.654	31.876		49.81
_	ATOM	1714		WAT		64		13.203	8.179	28.792		50.30
	ATOM	1715		TAW		65		21.887	5.385	43.977		50.58
	ATOM	1716	OWO	WAT	W	66		24.468	6.206	27.276	1.00	50.23

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	MOTA	1717	OWO	WAT	w 67	16.159 -6.928	39.274 1.00 50.79
	ATOM	1718	OWO	WAT	w 68	18.759 17.803	28.696 1.00 50.80
	MOTA	1719	OWO	WAT	W 69	13.821 14.472	25.933 1.00 52.01
	MOTA	1720	OWO	WAT	¥ 70	5.992 2.145	
5	MOTA	1721	OWO	WAT	W 71	22.450 0.866	42.331 1.00 52.86
	MOTA	1722	OWO	WAT	v 72	37.480 14.455	29.856 1.00 52.16
	MOTA	1723	OWO	TAW		7.914 14.799	
	MOTA	1724	OWO	WAT !		33.074 14.728	12.928 1.00 52.80
• •	ATOM	1725		WAT		-2.139 5.177	35.817 1.00 53.07
10	MOTA	1726		WAT		8.849 6.339	29.567 1.00 53.08
	MOTA	1727		WAT		2.499 9.596	40.507 1.00 53.22
	MOTA	1728		WAT		8.453 -4.313	50.928 1.00 53.22
	MOTA	1729		WAT		13.988 -16.279	37.477 1.00 54.52
1.5	ATOM	1730		WAT		29.311 23.613	25.169 1.00 53.94
15	MOTA	1731		WAT		10.698 17.607	37.556 1.00 53.87
	ATOM	1732		WAT		10.533 -28.803	42.420 1.00 54.34
	ATOM	1733		WAT		1.674 -0.659	35.990 1.00 54.11
	MOTA	1734		WAT	_	13.238 5.649	29.129 1.00 54.35
20	ATOM	1735		VAT V		23.172 23.184	42.047 1.00 53.98
20	ATOM	1736		WAT V		25.591 -14.157	41.467 1.00 54.33
	ATOM	1737		WAT		39.505 4.678	27.285 1.00 55.10
	MOTA	1738		WAT		33.071 24.177	22.504 1.00 53.92
	ATOM	1739		WAT		2.865 -14.306	47.361 1.00 55.09
25	ATOM	1740		WAT		10.824 5.199	27.990 1.00 54.87
23	ATOM	1741		WAT		13.268 -18.762	37.013 1.00 55.07
	ATOM	1742		WAT		19.672 23.135	34.883 1.00 56.03
	MOTA	1743	_	WAT V		3.899 3.408 17.326 5.781	32.498 1.00 56.24 50.106 1.00 56.35
	ATOM	1744		WAT W		17.326 5.781 46.420 28.753	50.106 1.00 56.35 20.001 1.00 56.50
30	ATOM ATOM	1745 1746		WAT V		18.033 -25.950	38.021 1.00 56.78
50	ATOM	1747		WAT V		16.668 11.173	20.729 1.00 57.28
	ATOM	1748		WAT		-0.327 -1.130	37.865 1.00 56.31
	ATOM	1749		WAT V		13.791 -29.887	42.473 1.00 56.28
	ATOM	1750			100	14.138 -6.120	36.256 1.00 56.78
35	ATOM	1751		WAT W		-0.503 -1.004	43.200 1.00 56.68
55	ATOM	1752			102	7.034 2.268	29.920 1.00 57.78
	ATOM	1753	OWO		103	39.612 16.983	21.840 1.00 57.56
	ATOM	1754		WAT W		12.322 -7.683	34.772 1.00 57.82
	ATOM	1755			105	21.186 21.778	39.197 1.00 58.10
40	ATOM	1756		WAT W		25.213 27.127	14.493 1.00 58.04
	ATOM	1757		WAT W		37.189 5.450	11.613 1.00 58.31
	ATOM	1758		WAT W		25.799 -17.600	47.916 1.00 58.58
	ATOM	1759		WAT W		25.505 0.503	36.518 1.00 57.70
	ATOM	1760		WAT W		21.154 19.292	24.315 1.00 58.80
45	ATOM	1761		WAT W		23.932 23.123	29.269 1.00 58.45
	ATOM	1762		WAT W		30.025 16.034	12.701 1.00 58.92
	ATOM	1763	OWO	WAT W	113	5.440 -12.369	36.445 1.00 60.00
	ATOM	1764	OWO	WAT W	114	45.949 18.908	19.720 1.00 59.22
	ATOM	1765	OWO	WAT W	115	3.882 16.171	43.893 1.00 59.38
50	ATOM	1766	OWO	WAT W	116	26.040 -17.629	41.513 1.00 58.92
	MOTA	1767	OWO	WAT W	117	13.942 -10.256	37.298 1.00 60.39
	ATOM	1768	OWO	WAT W	118	7.840 10.062	31.734 1.00 60.14
	MOTA	1769	OW0	WAT W	119	-1.860 -20.559	43.212 1.00 60.45
	ATOM	1770	OWO	WAT W	120	18.311 16.851	47.879 1.00 60.32
55	ATOM	1771	OWO	WAT W	121	38.093 15.693	26.658 1.00 61.27
	ATOM	1772		WAT W		7.557 -26.418	44.769 1.00 61.39
	MOTA	1773		WAT W		17.200 -4.612	32.783 1.00 60.41
	MOTA	1774		WAT W		33.055 , 9.791	13.378 1.00 61.34
	ATOM	1775		WAT W		29.579 10.149	37.422 1.00 60.84
60	MOTA	1776		WAT W		26.196 13.297	42.367 1.00 60.80
	ATOM	1777		WAT W		23.556 -4.737	42.642 1.00 61.18
	ATOM	1778		WAT W		10.687 -3.375	35.374 1.00 61.88
	ATOM	1779	OWO	WAT W	129	13.030 -13.947	38.339 1.00 62.52

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	ATOM	1780	OWO	WAT	W	130	9.747 -0.992	36.212	1.00 59.32
	ATOM	1781	OWO	WA 1	W	131	24.814 -11.997	45.661	1.00 62.19
	ATOM	1782	OWO	raw .	' W		23.200 4.574	23.546	1.00 61.90
_	MOTA	1783	OWO				24.938 30.370	17.496	1.00 62.23
5	MOTA	1784	OWO				35.459 1.260	16.603	1.00 62.66
	ATOM	1785		WA 1			24.178 20.068	20.090	1.00 61.73
	ATOM	1786	OWO			-	40.127 0.350	18.771	1.00 62.44
	MOTA	1787		WAI			19.279 14.663	46.778	1.00 63.59
10	MOTA		- OMO				20.090 20.354	46.023	1.00 62.81
10	ATOM	1789	OWO				15.250 18.974	46,516	1.00 63.68
	ATOM	1790	OWO				21.267 -25.030	39.386	1.00 63.31
	ATOM	1791		WAT			26.107 2.756	33.033	1.00 63.89
	ATOM	1792		TAW			13.216 16.259	48.398	1.00 64.51
16	ATOM	1793		WAT			23.474 19.596	51.112	1.00 65.45
15	ATOM	1794	OWD				6.778 10.141	28.981	1.00 64.57
	MOTA	1795		TAW			23.613 15.848	49.685	1.00 64.50
	MOTA	1796		WAT			21.834 -6.518	36.556	1.00 65.24
	ATOM	1797		TAW			10.139 -10.444	36.806	1.00 65.85
20	ATOM	1798		WAT			32.489 10.232	33.677	1.00 64.60
20	ATOM	1799		TAW		149	31.655 6.263	27.510	1.00 64.29
	ATOM	1800		TAW			4.585 -20.934	39.031	1.00 66.94
	MOTA	1801		TAW		151	38.484 11.674	18.085	1.00 65.84
	MOTA	1802		WAT		152	42.438 8.992	21.219	1.00 65.71
25	ATOM	1803		WAT		153	33.971 24.173	27.259	1.00 66.15
25	MOTA	1804		WAT		154	24.597 -9.268	45.286	1.00 67:06
	ATOM	1805		WAT		155	-2.112 -26.008	50.039	1.00 66.08
	ATOM	1806		WAT		156	9.030 -32.481	39.896	1.00 66.14
	MOTA	1807		WAT		157	-3.216 -18.835	45.004	1.00 67.94
30	ATOM	1808		WAT			-3.398 4.020	40.260	1.00 65.32
30	MOTA	1809		WAT		159	25.878 24.231	20.622	1.00 68.10
	MOTA	1810	-	WAT		160	27.187 4.546	24.805	1.00 67.75
	ATOM	1811		WAT		161	24.071 24.303	35.784	1.00 67.51
	MOTA	1812	OWO	WAT		162	7.746 17.585	52.663	1.00 70.19
35	ATOM	1813		WAT		163	19.301 4.980	47.873	1.00 68.23
33	ATOM	1814		WAT		164	10.439 -4.135	32.539	1.00 65.45
	ATOM	1815		WAT	W	165	23.798 -0.930	41.113	1.00 68.64
	ATOM	1816	OWO	WAT			2.464 5.318	30.549	1.00 65.77
	ATOM ATOM	1817 1818		WAT	W	167 168	9.665 -14.876	35.700	1.00 65.21
40	ATOM	1819				169	1.759 10.431 20.960 4.214	44.227	1.00 69.25
40	ATOM	1820	OWO	WAT	W	170		26.258	1.00 69.97
	ATOM	1821		WAT		171	28.769 24.807 30.212 14.473	27.878 8.293	1.00 67.86 1.00 69.23
	ATOM	1822		WAT		172	20.178 0.312	50.589	
	ATOM	1823		WAT	M	173	19.736 6.852	23.117	1.00 70.29 1.00 70.72
45	ATOM	1824	OWO		W	174	8.978 16.807	50.514	1.00 70.72
45	ATOM	1825	OWO	WAT	W	175	25.144 -1.759	34.429	1.00 70.10
	ATOM	1826		WAT		176			1.00 71.96
		1827				177		35,563	
	ATOM ATOM	1828		WAT	W	178	44.918 5.619 22.370 24.094	13.054 38.170	1.00 70.16 1.00 71.66
50	MOTA	1829	OWO	WAT		179	~0.624 10.187	38.170	1.00 71.66
-0	ATOM	1830	OWO	WAT		180	11.015 17.856	47.520	1.00 72.23
	ATOM	1831	OWO	WAT		181	7.766 0.898	52.950	1.00 71.42
	ATOM	1832		WAT			3.469 -28.368		1.00 71.64
	AIUN	1034	OWU	AALT	W	102	3.403 -20.300	52.511	1.00 /0.10

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Claims

- 5 1. A crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein or homologue thereof, comprising residues vital for transcriptional and replicational activities of said protein.
- 2. An E2NT dimer protein according to Claim 1 wherein the residues lie on opposite sides of an N-terminal domain.
 - 3. An E2NT dimer protein according to either preceding claim wherein the residues comprise a plurality of residue clusters associated with a structural role at an interface between N1 and N2 terminal domains of respective monomers within the dimer.
 - 4. An E2NT dimer according to Claim 3 comprising three clusters.
- 5. An E2NT dimer according to either of Claims 3 or 4 wherein a first cluster of vital residues is associated with interactions between N1 and N2 domains and comprises any one or more of the following residues Ile82, Glu90, Trp92, Lys112, Tyr138, Val145.
- An E2NT dimer according to any one of Claims 3-5 wherein a second cluster
 of residues is associated with N1 interactions and comprises either or both of residues
 Trp33 and Leu94.
 - 7. An E2NT dimer according to any one of Claims 3-6 wherein a third cluster of residues is associated with N2 interactions and comprises any one or more of the following residues Pro106, Lys111, Phe168, Trp134.

8. An E2NT dimer according to any preceding claim further comprising residues associated with transactivation and/or replication properties of E2.

9. An E2NT dimer according to Claim 8 wherein the residues comprise any one or more of the following residues Glu20, Glu100, Asp122, Arg37, Glu39, Ile73, Gln12 and Ala69.

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- 10. Use of a crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein according to any preceding claim or homologue thereof in mapping mutations onto an E2 three-dimensional structure so as to identify areas of amino acid conservation and the effect of mutations on folding of the E2 protein.
 - 11. Use according to Claim 10 in rationalised antiviral drug design.
- 15 12. An *in vitro* method for identifying and/or selecting a candidate therapeutic agent, the method comprising determining interaction of a E2 N-terminal module (E2NT) dimer in a sample by contacting said sample with said candidate therapeutic agent and measuring DNA loop formation in E2.
- 20 13. Use of the method according to Claim 12 in identifying and/or selecting an antiviral candidate therapeutic agent.
- 14. Use according to Claim 13 wherein identification/selection of the candidate therapeutic agent depends on its ability to interfere with or block interactions of
 E2NT so as to interfere or block viral and/or cellular transcription factors.
 - 15. Use of an E2NT dimerisation inhibitor for the preparation of a medicament for treatment of conditions that arise as a result of HPV infection.
- 30 16. Use according to Claim 15 for the treatment of warts, proliferative skin lesions and/or cervical cancer.

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17. A method of monitoring the efficacy of an antiviral therapy in a patient receiving a medicament for the treatment of an HPV infection comprising taking a sample from said patient and measuring E2NT interactions and/or DNA loop formation.

- 18. Use of a dimerisation surface of an crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein or homologue thereof according to any one of Claims 1-9 as a target site for interaction with putative antiviral agents and/or for measuring efficacy of said agents.
- 19. A method for identifying and/or selecting a candidate therapeutic agent, comprising applying rationalised drug design to a crystal structure obtainable by crystallising E2NT, cryogenically freezing the crystals and generating the crystal structure using X-ray diffraction.
- 20. A method of claim 19, wherein the method by which the E2NT crystal structure is obtainable comprises crystallisation using hanging-drop vapour diffusion.
- 20 21. A method of claim 19 or claim 20 wherein the method by which E2NT crystal structure is obtainable comprises X-ray diffraction using uranium acetate and gold cyanide E2NT derivatives and refining with data extending to 1.9 Å spacing.
- A method of any of claims 19 to 21, wherein the crystal structure comprises
 the portions of amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94.
 - 23. A method of any of claims 19 to 22, wherein the rationalised drug design comprises designing drugs which interact with the dimerisation surface of E2NT.
 - 24. A computer for producing a three-dimensional representation of a molecule or molecular complex, wherein said molecule or molecular complex comprises or a

three-dimensional representation of a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å, wherein said computer comprises:

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(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises the structure coordinates of E2NT amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94 according to Table 3;

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(b) a working memory for storing instructions for processing said machine-readable data;

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(c) a central-processing unit coupled to said working memory and to said machine readable data storage medium for processing said machine readable data into said three-dimensional representation; and

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- (d) a display coupled to said central-processing unit for displaying said threedimensional representation.
- 25. The computer according to claim 24, wherein said three-dimensional representation is of a molecule or molecular complex is defined by the set of structure coordinates according to Table 3, or wherein said three-dimensional representation is of a homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said
- amino acids of not more than 1.5 Å.
 - 26. A computer for determining at least a portion of the structure coordinates corresponding to an X-ray diffraction pattern of a molecule or molecular complex, wherein said computer comprises:

(a) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises at least a portion of the structural coordinates according to Table 3;

- (b) a machine-readable data storage medium comprising a data storage material encoded with machine-readable data, wherein said data comprises an X-ray diffraction pattern of said molecule or molecular complex;
- (c) a working memory for storing instructions for processing said machine-readable data of (a) and (b);
 - (d) a central-processing unit coupled to said working memory and to said machinereadable data storage medium of (a) and (b) for performing a Fourier transform of the machine readable data of (a) and for processing said machine readable data of (b) into structure coordinates; and

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- (e) a display coupled to said central-processing unit for displaying said structure coordinates of said molecule or molecular complex.
- 27. A crystallised molecule or molecular complex comprising a dimerisation surface defined by structure coordinates of E2NT amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94 according to Table 3or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.
 - 28. The crystallized molecule or molecular complex according to claim 27, wherein said molecule or molecular complex is defined by the set of structure coordinates according to Table 3, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

29. A machine-readable data storage medium, comprising a data storage material encoded with machine readable data which, when using a machine programmed with instructions for using said data, is capable of displaying a graphical three-dimensional representation of a molecule or molecular complex comprising a dimerisation surface defined by structure coordinates of E2NT amino acids Ile82, Glu90, Trp92, Lys112, Tyr138, Val145, Pro106, Lys111, Phe168, Trp134, Trp33 and Leu94 according to Table 3, or a homologue of said molecule or molecular complex, wherein said homologue comprises a binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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30. The machine-readable data storage medium according to claim 7, wherein said molecule or molecular complex is defined by the set of structure coordinates according to Table 3, or a homologue of said molecule or molecular complex, said homologue having a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å.

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31. A machine-readable data storage medium comprising a data storage material encoded with a first set of machine readable data which, when combined with a second set of machine readable data, using a machine programmed with instructions for using said first set of data and said second set of data, can determine at least a portion of the structure coordinates corresponding to the second set of machine readable data, wherein: said first set of data comprises a Fourier transform of at least a portion of the structural coordinates according to Table 3; and said second set of data comprises an x-ray diffraction pattern of a molecule or molecular complex.

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32. A method for evaluating the ability of a chemical entity to associate with a molecule or molecular complex according to claim 27 or claim 28 comprising the steps of:

a. employing computational means to perform a fitting operation between the chemical entity and a dimerisation surface of the molecule or molecular complex; and

b. analysing the results of said fitting operation to quantify the association between the chemical entity and the dimerisation surface.

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33. A drug or therapeutic agent identified, assessed or selected using a crystallised molecular complex of an E2NT protein or its crystal structure or using a complex of any of claims 1 to 9, a method of claim 12, a use of any of claims 13, claim 14 or 18. a method of any of claims 20 to 24 or 32 or a product of any of claims 25 to 31.

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(71) Applicant (for all designated States except US): THE UNIVERSITY OF YORK [GB/GB]; Heslington Hall, York YO10 5DD (GB).

(72) Inventors; and

(75) Inventors/Applicants (for US only): ANTSON, Alfred [GB/GB]; Department of Chemistry, University of York, York YO10 5DD (GB). MAITLAND, Norman [GB/GB]; Department of Biology, University of York, York YO10 5DD (GB).

(74) Agent: HARRISON GODDARD FOOTE; Tower House, Merrion Way, Leeds LS2 8PA (GB).

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(54) Title: TARGET FOR ANTIVIRAL THERAPY

(57) Abstract: A crystallised molecular complex of an E2 N-terminal module (E2NT) dimer protein or homologue thereof, that comprises residues vital for viral transcription and/or replication. The invention also provides for the use of the dimer protein and interactions at its dimerisation surface in rationalised antiviral drug design.

FIG. I. A

HPV 16 E2 Protein: Functional assignments

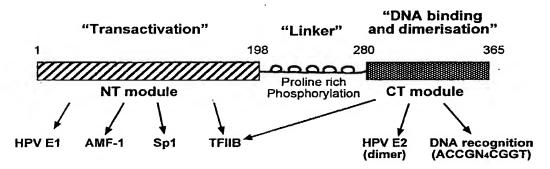
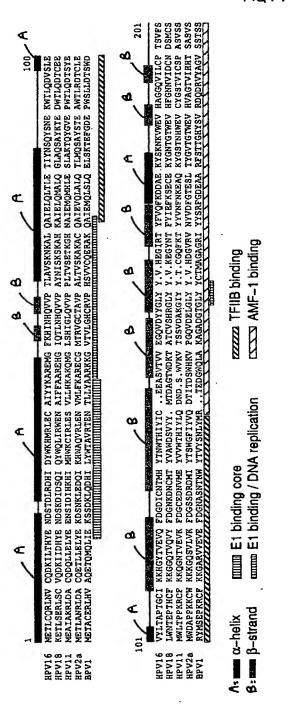
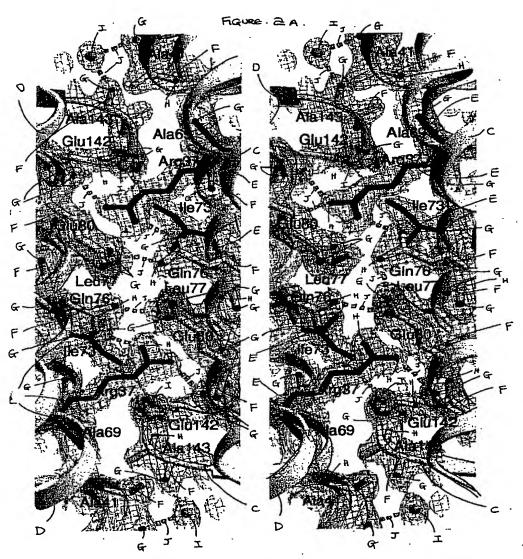


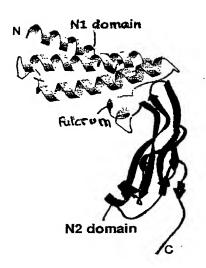
Fig. 1. B

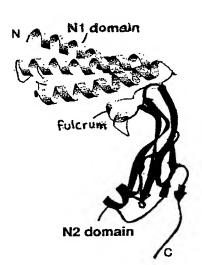




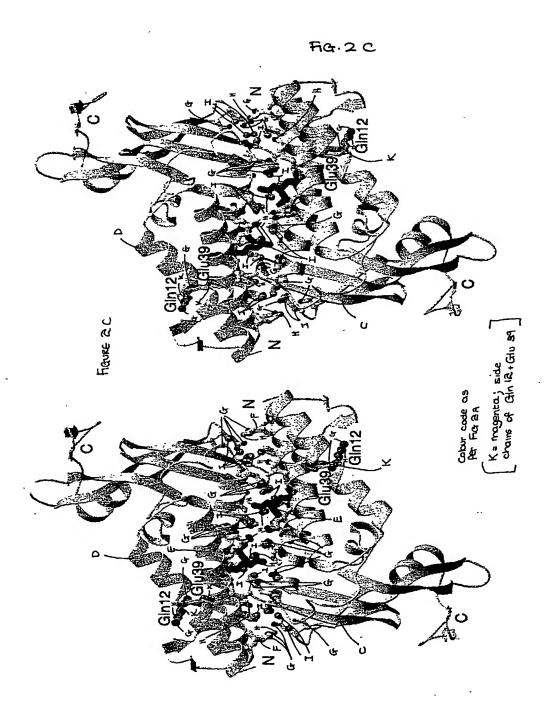
C. blue; monomer ribbon: D= yellow; monomer ribbon: E. dark green; side chause of Arg37 and Ile 73; F = light green; side chause of other residues: G = O2; red: H = blue; N2; I = orange 1120: J = dashod sticks; hydrogen bonds]

tique . 2 B





N = N1 domain = a quamorine M = fulcrum = qreen L = N2 domain = pink



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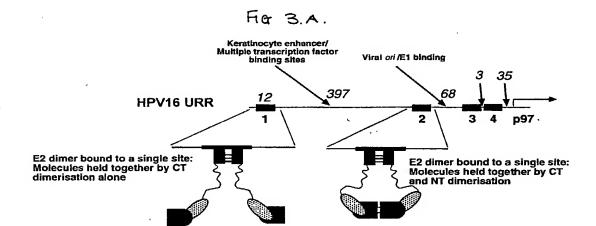


FIG. 3B

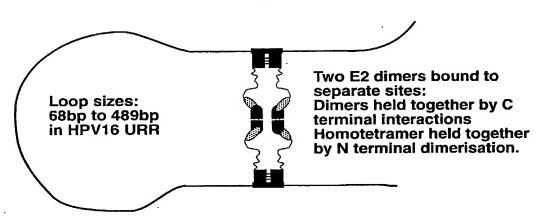
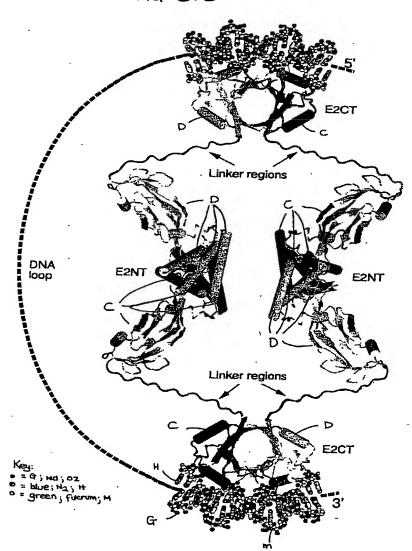
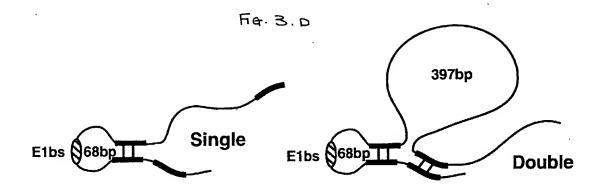


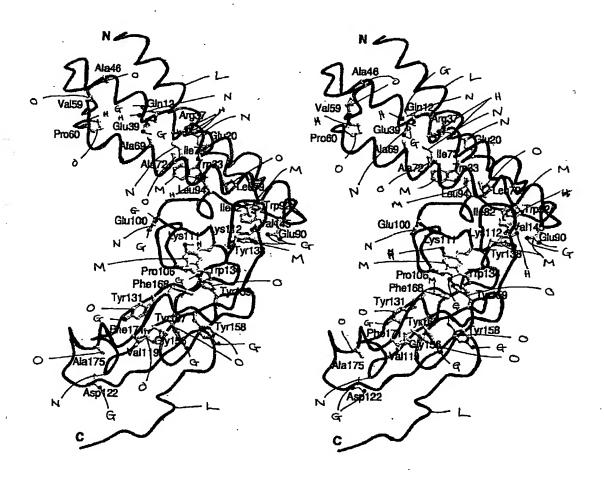
Fig. 3. C





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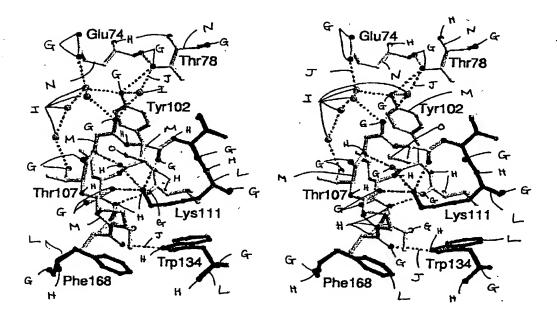
Fig. 4 A.



0 = yellow; sulphur atoms.

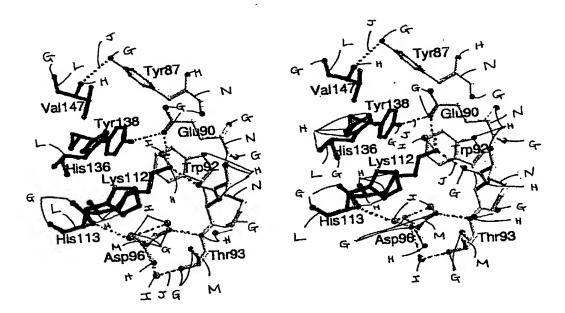
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Fig. 4.B



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Fig. 4C



Flaure 4D.

DECLARATION AND POWER OF ATTORNEY FOR PATENT APPLICATION Attorney Docket No. 9052-111

As a below named inventor, I hereby declare that:

My residence, post office address and citizenship are as stated below next to my name.

I believe I am the original, first and sole inventor (if only one name is listed below) or an original, first and joint inventor (if plural names are listed below) of the subject matter which is claimed and for which a patent is sought on the invention entitled **TARGET FOR ANTIVIRAL THERAPY**,

the specification of which
is attached hereto
OR
was filed on September 18, 2002 as United States Application No. or PCT International
Application Number PCT/GB00/03568 and was amended on (if applicable).
I hereby state that I have reviewed and understand the contents of the above-identified specification, including the claims, as amended by any amendment referred to above.

I acknowledge the duty to disclose information which is material to patentability as defined in Title 37 Code of Federal Regulations, §1.56, including material information that became available between the filing date of the prior application and the National or PCT International filing date of the continuation-in-part application, if applicable.

I hereby claim foreign priority benefits under Title 35, United States Code, § 119(a)-(d) or § 365(b) of any foreign application(s) for patent or inventor's certificate, or § 365(a) of any PCT International application which designated at least one country other than the United States of America, listed below and have also identified below any foreign application for patent or inventor's certificate, or of any PCT International application having a filing date before that of the application on which priority is claimed.

9921938.8	Great Britain	09/17/1999	⊠ Yes □ No
Number	Country	MM/DD/YYYY Filed	Priority Claimed
			☐ Yes ☐ No
Number	Country	MM/DD/YYYY Filed	Priority Claimed
			☐ Yes ☐ No
Number	Country `	MM/DD/YYYY Filed	Priority Claimed

Page 1 of 4

I hereby claim the benefit under Title 35, United States Code, § 119(e) of any United States provisional application(s) listed below.

None	
Application Number(s)	Filing Date (MM/DD/YYYY)

I hereby claim the benefit under Title 35, United States Code, § 120 of any United States application(s) or § 365(c) of any PCT international application designating the United States of America, listed below.

PCT/GB00/03568 Appln. Serial No.	09/18/00 Filing Date	Published Status Patented/Pending/Abandoned
Appln. Serial No.	Filing Date	Status Patented/Pending/Abandoned
Appln. Serial No.	Filing Date	Status Patented/Pending/Abandoned

I hereby declare that all statements made herein of my own knowledge are true and that all statements made on information and belief are believed to be true; and further that these statements were made with the knowledge that willful false statements and the like so made are punishable by fine or imprisonment, or both, under Section 1001 of Title 18 of the United States Code and that such willful false statements may jeopardize the validity of the application or any patent issued thereon.

POWER OF ATTORNEY: As a named inventor, I hereby appoint the following registered attorney(s) to prosecute this application and transact all business in the Patent and Trademark Office connected therewith. I also appoint the following registered attorney(s) to represent me before all competent International Authorities in connection with any and all international applications filed by me with an appropriate receiving office claiming priority to the U.S.



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Customer Number:



Send correspondence to:

Jarett K. Abramson **Customer Number:**

20792 PATENT TRADEMARK OFFICE

Direct telephone calls to:

Jarett K. Abramson

(919) 854-1400

Facsimile:

(919) 854-1401

Full name of first inventor:

Alfred Antson

Inventor's

Signature:

Date: 67.05.07

Residence:

York, Great Britain, United Kingdom

Citizenship:

Great Britain

Mailing Address:

Department of Chemistry

University of York

York YO10 5DD, Great Britain

United Kingdom

2-00

Full name of second inventor:

Norman Maitland

Inventor's

Signature: Mma

Date:

105/02

Residence:

York, Great Britain, United Kingdom

Citizenship:

Great Britain

GB

Mailing Address:

Department of Biology University of York

YO10 5DD, Great Britain

United Kingdom